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K3. AN EULERIAN FINITE DIFFERENCE PROGRAM FOR THREE-DIMENSIONAL--ETC(U)
FEB 80 J MAY, P SNOW, D C WILLIAMS DAS660-79-C-0098
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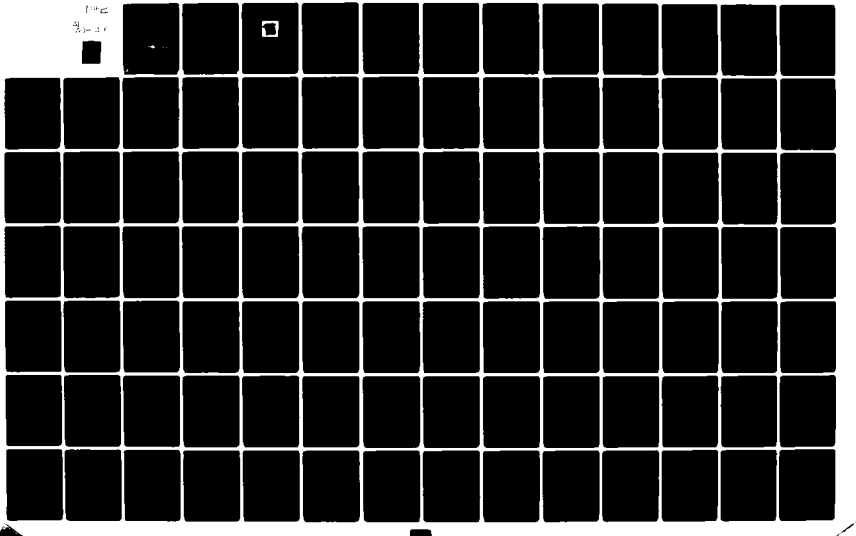

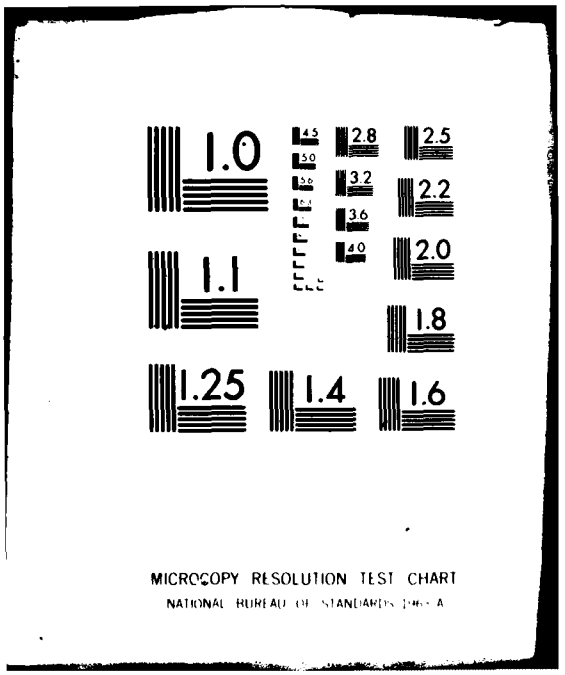
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K-80-226U(R)

K3 - AN EULERIAN FINITE DIFFERENCE PROGRAM FOR THREE-DIMENSIONAL MATERIAL RESPONSE

28 FEBRUARY 1980

FINAL REPORT

ADA087416

Sponsored by
The Ballistic Missile Defense Advanced Technology Center

KAMAN SCIENCES CORPORATION
1500 Garden of the Gods Road
Colorado Springs, Colorado 80907

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CSQII

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K3 IS A COMPUTER CODE FOR SIMULATION OF TARGET RESPONSE TO PROJECTILE IMPACTS. IT IS A THREE-DIMENSIONAL CODE DERIVED FROM CSQII, USED TO INVESTIGATE IMPACT LETHALITY PHENOMENA. A LAGRANGIAN-EULERIAN FINITE DIFFERENCE METHOD IS USED FEATURING A REZONING TECHNIQUE WITH RETENTION OF VOID VOLUMES. THIS MANUAL PROVIDES THE TECHNICAL INFORMATION REQUIRED TO UNDERSTAND THE CSQII TO K3 EXTENSION AND DETAILS THE INPUTS NECESSARY FOR PROGRAM EXECUTION, AS WELL AS PROVIDING EXAMPLE CALCULATIONS.

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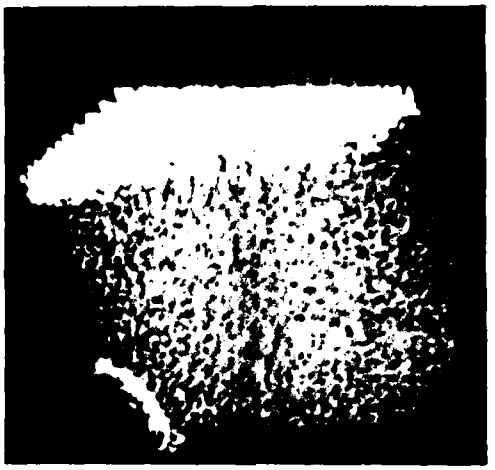

KAMAN SCIENCES CORPORATION
1500 GARDEN OF GODS ROAD
COLORADO SPRINGS CO. 80907

28 FEBRUARY 1980

FINAL REPORT

DASG 60-79-C-0098

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PREFACE

Ballistic Missile Defense impact lethality problems involving non-nuclear kill mechanisms and fragment damage processes have become increasingly complex. Complicated target configurations, extreme impact conditions, and varying angles of attack require the use of sophisticated computer simulations to model problem geometries. Several different hydrocodes have been used, but where complicated geometry existed, modifications have had to be made to the configuration to fit the constraints of the codes. In order to analyse these problems without the need of bending the problem to fit the code, it was decided to construct a new code that would handle these configurations without alteration. Rather than develop a new code from scratch, an existing two-dimensional code was chosen as a foundation, where previous work and experience could be built upon. Since in previous work with two-dimensional hydrocodes, it was determined that one code, CSQII, performed better than others in correlating with test results, it was decided to use this code as a base. The result was K3, a computer code which simulates material response in three-dimensions. This report provides the technical information required to understand the CSQII to K3 extension, details the inputs and co trol cards necessary for execution on a CDC-7600, and presents the results from program development and checkout.

The authors wish to extend special thanks to Mr. S.L. Thompson of Sandia Laboratories for his ideas and comments during the development of K3. His help greatly aided the designers and shortened the K3 development period. Also, the authors are indebted to the many people who contributed to the K3 effort by providing help in debugging the code.

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I INTRODUCTION

K3 is a computer code developed by Kaman Sciences Corporation under contract to the Ballistic Missile Defense Advanced Technology Center for the simulation of three-dimensional material motion. K3 is an extension of CSQ, a program for computation of two-dimensional material motion developed by Sandia Laboratories, Albuquerque, New Mexico. The form of CSQ has been retained in the computational method, input and output form and in the names of subroutines. A familiarity with CSQ would greatly aid the users of K3 since the basic material explaining many concepts common to the two codes is not repeated here. Rather, it is the intent of this report to present where and why modifications have been made in order to make the extension to the third dimension. Users should note that the K3 program is not perfectly clean in the sense that all program references to "CSQ" have been converted to "K3". The development of K3 is an ongoing task where improvements are continually being made. In the course of this work it is hoped that eventually K3 will cease to be a hybrid and will become a unique program.

K3 is a title that applies both to a program and to the package of programs which include and support K3. The support programs are

PREK3	-	generates the COMDECKs used by other programs in the package
K3GEN	-	generates the K3 (re)start tape from the initial problem configuration
K3PLT	-	graphics program for plotting K3 results

Other programs which are part of the CSQ package but not listed here have not yet been converted to the K3 system. Also, several capabilities of CSQ have yet to be included within the K3 programs. These include

- cylindrical geometry
- rezone/remeshing operations
- energy sources
- high explosives

- tracer particles
- radiation
- various plot options in K3PLT

Wherever possible, these CSQ capabilities which are embodied in specific subroutines have been retained pending future conversion and modification efforts. Since these routines still exist in the code, it is theoretically possible to execute these capabilities, but since results are neither known nor guaranteed, use of these capabilities is highly discouraged. Wherever certain inputs could route the execution path through unmodified portions of the code, comments are included to warn the user that only the K3 standard input values should be defined.

This report is divided into these main parts: Part I, Introduction; Part II, Sections A and B, is intended to aid those users interested in the physical considerations inherent in the K3 code. Section A presents, without derivation, some of the more important modified and generalized equations which form the basis of the K3 program. Section B attempts to give the user an understanding of how the physical laws governing material flow are incorporated into K3 through use of finite difference relationships and the spatial mesh. Though it is not necessary for the user to understand the equations presented or the code structure to successfully use the K3 program, a review of the material of these sections should be made for better understanding the necessary inputs and the resultant outputs. The next part is a programmers guide presenting a description of the restart tape and COMMON blocks for use by users who wish to modify the program.

Section IV is a user's guide, with a listing of control cards necessary for code execution (Section A), and inputs for the programs in the K3 package (Section B). Appendix A gives a brief overview of the procedures used and results obtained in the course of K3 program development, test and debug.

II PHYSICAL AND NUMERICAL RELATIONSHIPS

A. PHYSICAL RELATIONSHIPS

1. Conservation Equations

The Lagrangian forms of the conservation laws in Cartesian coordinates which control the three dimensional flow of substances in K3 are as follows:

Conservation of Mass

$$-\frac{1}{\rho}\frac{\partial \rho}{\partial t} = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z} \tag{2.1}$$

Conservation of Momentum

$$-\rho \frac{\partial V_x}{\partial t} = \frac{\partial}{\partial x}(\sigma_{xx} + P_r + Q_{xx}) + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \tag{2.2}$$

$$-\rho \frac{\partial V_y}{\partial t} = \frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial}{\partial y}(\sigma_{yy} + P_r + Q_{yy}) + \frac{\partial \sigma_{yz}}{\partial z} \tag{2.3}$$

$$-\rho \frac{\partial V_z}{\partial t} = \frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{zy}}{\partial y} + \frac{\partial}{\partial z}(\sigma_{zz} + P_r + Q_{zz}) \tag{2.4}$$

Conservation of Energy

$$\frac{\partial}{\partial t}\left(E_m + \frac{E_r}{\rho}\right) = -(P_m + P_r + \tilde{Q})\frac{\partial}{\partial t}\left(\frac{1}{\rho}\right) - \frac{1}{\rho}\nabla \cdot \bar{F} + \dot{\xi} + P_d \tag{2.5}$$

In the preceding conservation equations t denotes time and ρ denotes density. Assuming that the index notation i = 1, 2, 3 corresponds to Cartesian coordinates x, y, z, then V_i, σ_{ij} and Q_{ij} denote the velocity, stress tensor and artificial

viscosity tensor components, respectively. The notation pertaining to the remaining variables is as follows:

E_m - specific material internal energy

E_r - radiation energy density

P_d - stress deviator power

P_m - material pressure

P_r - radiation pressure

$\tilde{Q}$ - artificial viscosity quantity (Section II-A-2)

$\overline{F}$ - energy flow flux vector

$\dot{s}$ - specific internal energy production rate

The three dimensional conservation laws can be rewritten like those pertaining to CSQ. The procedure for rewriting these equations is contained in Section II-1, Reference 1.

2. Artificial Viscosity

The conservation of mass equation (2.1) can be written as

$$-\frac{1}{\rho}\frac{\partial \rho}{\partial t} = \nabla \cdot \overline{V} = \tilde{f}_x + \tilde{f}_y + \tilde{f}_z \qquad (2.6)$$

where

$$\tilde{f}_x = \frac{\partial V_x}{\partial x} \qquad \tilde{f}_y = \frac{\partial V_y}{\partial y} \qquad \tilde{f}_z = \frac{\partial V_z}{\partial z} \qquad (2.7)$$

The generalization of the CSQ viscosity tensor to three dimensions using (2.7) is as follows. Define

$$f_x = \tilde{f}_x \qquad \text{if } \tilde{f}_x < 0$$

$$= 0 \qquad \text{if } \tilde{f}_x \geq 0 \tag{2.8}$$

$$f_y = \tilde{f}_y \qquad \text{if } \tilde{f}_y < 0$$

$$= 0 \qquad \text{if } \tilde{f}_y \geq 0 \tag{2.9}$$

$$f_z = \tilde{f}_z \qquad \text{if } \tilde{f}_z < 0$$

$$= 0 \qquad \text{if } \tilde{f}_z \geq 0 \tag{2.10}$$

With these functions the diagonal elements of the artificial viscosity tensor are nonzero when the material is undergoing compression and are given by

$$Q_{xx} = \rho\left[B_q^2(f_x + f_y + f_z) - B_\ell C_s\right]f_x \tag{2.11}$$

$$Q_{yy} = \rho\left[B_q^2(f_x + f_y + f_z) - B_\ell C_s\right]f_y \tag{2.12}$$

$$Q_{zz} = \rho\left[B_q^2(f_x + f_y + f_z) - B_\ell C_s\right]f_z \tag{2.13}$$

where B_ℓ and B_q are constants.

The artificial viscosity tensor components Q_{xy}, Q_{yx}, Q_{xz}, Q_{zx}, Q_{yz} and Q_{zy} are all zero in the K3 program. The quantity $\tilde{Q}$ in equation (2.5) is

$$\tilde{Q} = \frac{Q_{xx}f_x + Q_{yy}f_y + Q_{zz}f_z}{f_x + f_y + f_z} \tag{2.14}$$

CSQ has the capability to use viscosity which operates in expansion as well as in compression. This capability is in K3 and can be activated using variable ARRX(12) in the ARRX array.

In CSQ it is optional whether the sound speed is retained in the main storage arrays. This feature is retained in K3. Whenever the sound speed C_s is not available for use in the viscosity sections of the program, it is approximated by

$$C_s = \text{Max}\left[C_{i_{ref}}, \sqrt{\frac{\delta P}{\rho}}\right] \tag{2.15}$$

where $C_{i_{ref}}$ is the reference point and sound speed for material i. Here P and ρ are cell variables and $\delta = 5/3$. The values of $C_{i_{ref}}$ and δ can be changed per ARRX(47) and ARRX(48) in the ARRX array.

3. Elastic-Plastic Materials

The physical relations pertaining to the elastic-perfectly plastic model in CSQ are presented in Section II-4 of Reference 1. Only those relations that were extended for the K3 model are given in the subsequent discussion.

The independent elements of the stretching tensor are

$$d_{xx} = \frac{\partial V_x}{\partial x} \tag{2.16}$$

$$d_{yy} = \frac{\partial V_y}{\partial y} \tag{2.17}$$

$$d_{zz} = \frac{\partial V_z}{\partial z} \tag{2.18}$$

$$d_{xy} = d_{yx} = \frac{1}{2}\left(\frac{\partial V_x}{\partial y} + \frac{\partial V_y}{\partial x}\right) \tag{2.19}$$

$$d_{xz} = d_{zx} = \frac{1}{2}\left(\frac{\partial V_x}{\partial z} + \frac{\partial V_z}{\partial x}\right) \tag{2.20}$$

$$d_{yz} = d_{zy} = \frac{1}{2}\left(\frac{\partial V_y}{\partial z} + \frac{\partial V_z}{\partial y}\right) \tag{2.21}$$

The volumetric strain rate or dilation rate is

$$d = d_{xx} + d_{yy} + d_{zz} = -\frac{1}{\rho}\frac{\partial \rho}{\partial t} \tag{2.22}$$

The stretching deviators are defined as

$$d^d_{xx} = d_{xx} - \frac{d}{3} \tag{2.23}$$

$$d^d_{yy} = d_{yy} - \frac{d}{3} \tag{2.24}$$

$$d^d_{zz} = d_{zz} - \frac{d}{3} \tag{2.25}$$

$$d^d_{yx} = d^d_{xy} = d_{xy} \tag{2.26}$$

$$d^d_{zx} = d^d_{xz} = d_{xz} \tag{2.27}$$

$$d^d_{zy} = d^d_{yz} = d_{yz} \tag{2.28}$$

The spin tensor components are

$$W_{xx} = W_{yy} = W_{zz} = 0 \tag{2.29}$$

$$W_{xy} = - W_{yx} = \frac{1}{2}\left(\frac{\partial V_x}{\partial y} - \frac{\partial V_y}{\partial x}\right) \tag{2.30}$$

$$W_{xz} = - W_{zx} = \frac{1}{2}\left(\frac{\partial V_x}{\partial z} - \frac{\partial V_z}{\partial x}\right) \tag{2.31}$$

$$W_{yz} = - W_{zy} = \frac{1}{2}\left(\frac{\partial V_y}{\partial z} - \frac{\partial V_z}{\partial y}\right) \tag{2.32}$$

The material pressure P is

$$P = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) \tag{2.33}$$

The components of the stress deviator tensor are

$$\sigma^d_{xx} = P - \sigma_{xx} \tag{2.34}$$

$$\sigma^d_{yy} = P - \sigma_{yy} \tag{2.35}$$

$$\sigma^d_{zz} = P - \sigma_{zz} \tag{2.36}$$

$$\sigma^d_{yx} = \sigma^d_{xy} = - \sigma_{xy} \tag{2.37}$$

$$\sigma^d_{zx} = \sigma^d_{xz} = - \sigma_{xz} \tag{2.38}$$

$$\sigma^d_{zy} = \sigma^d_{yz} = - \sigma_{yz} \tag{2.39}$$

Elastic changes in the stress deviators are given by

$$\frac{\partial \sigma^d_{xx}}{\partial t} - 2W_{xy}\sigma^d_{xy} - 2W_{xz}\sigma^d_{xz} = 2Gd^d_{xx} \tag{2.40}$$

$$\frac{\partial \sigma^d_{yy}}{\partial t} - 2W_{yx}\sigma^d_{yx} - 2W_{yz}\sigma^d_{yz} = 2Gd^d_{yy} \tag{2.41}$$

$$\frac{\partial \sigma^d_{zz}}{\partial t} - 2W_{zx}\sigma^d_{zx} - 2W_{zy}\sigma^d_{zy} = 2Gd^d_{zz} \tag{2.42}$$

$$\frac{\partial \sigma^d_{xy}}{\partial t} + W_{xy}(\sigma^d_{xx} - \sigma^d_{yy}) - W_{yz}\sigma^d_{xz} - W_{xz}\sigma^d_{yz} = 2Gd^d_{xy} \tag{2.43}$$

$$\frac{\partial \sigma^d_{xz}}{\partial t} + W_{xz}(\sigma^d_{xx} - \sigma^d_{zz}) - W_{zy}\sigma^d_{xy} - W_{xy}\sigma^d_{zy} = 2Gd^d_{xz} \tag{2.44}$$

$$\frac{\partial \sigma^d_{yz}}{\partial t} + W_{yz}(\sigma^d_{yy} - \sigma^d_{zz}) - W_{zx}\sigma^d_{yx} - W_{yx}\sigma^d_{zx} = 2Gd^d_{yz} \tag{2.45}$$

Here G is the shear modulus. Equations 2.40 - 2.45 can be derived from equation (6), P.445, Reference 2.

The preceding relations are valid whenever the material is in an elastic state. Whenever the material is no longer in an elastic state, stress deviators are calculated in K3 according to the preceding relations and then tested against a yielding criteria for plastic flow. The von Mises yield criteria used is

$$J_2' = \left[(\sigma^d_{xx})^2 + (\sigma^d_{yy})^2 + (\sigma^d_{zz})^2 + \sigma^d_{xx}\sigma^d_{yy} + \sigma^d_{xx}\sigma^d_{zz} + \sigma^d_{yy}\sigma^d_{zz} + (\sigma^d_{xy})^2 + (\sigma^d_{xz})^2 + (\sigma^d_{yz})^2\right] \leq \frac{Y}{3} \tag{2.46}$$

where J_2' is the second invariant of the stress sensor and Y is the yield stress. Whenever this inequality is not satisfied, the stress deviators are adjusted so that the stress state lies on the yield surface.

Equation (2.5) contains the deviator stress power P_d. It is given by

$$P_d = \frac{1}{\rho}\left[\sigma^d_{xx}d^d_{xx} + \sigma^d_{yy}d^d_{yy} + \sigma^d_{zz}d^d_{zz} + 2\sigma^d_{xy}d^d_{xy} + 2\sigma^d_{xz}d^d_{xz} + 2\sigma^d_{yz}d^d_{yz}\right] \tag{2.47}$$

4. Material Fracture

The K3 computation pertaining to fracture is such that when the pressure P is less than a fracture pressure $P_{fract} < 0$, void is introduced into the material. As in CSQ, there are two K3 options available for specifying P_{fract}. In one option P_{fract} is a user defined material constant. Fracture is based on principal stress values in the other option.

In CSQ the maximum and minimum normal principal stresses σ_1 and σ_2 are

$$\sigma_1 = \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) + t \tag{2.48}$$

$$\sigma_2 = \frac{1}{2}(\sigma_{xx} + \sigma_{yy}) - t \tag{2.49}$$

where

$$t = \sqrt{\left(\frac{\sigma_{xx} - \sigma_{yy}}{2}\right)^2 + \sigma_{xy}^2} \tag{2.50}$$

By placing a user specified bound σ_{fract} on σ_2 and using stress deviators, P_{fract} in CSQ is

$$P_{fract} = \sigma_{fract} + \frac{1}{2}(\sigma^d_{xx} + \sigma^d_{yy}) + \sqrt{\left(\frac{\sigma^d_{xx} - \sigma^d_{yy}}{2}\right)^2 + (\sigma^d_{xy})^2} \tag{2.51}$$

The computation for P_{fract} in K3 is

$$P_{fract} = \sigma_{fract} + \text{Max}\,[f_{xy}, f_{xz}, f_{yz}] \tag{2.52}$$

where

$$f_{xy} = \frac{1}{2}(\sigma^d_{xx} + \sigma^d_{yy}) + \sqrt{\left(\frac{\sigma^d_{xx} - \sigma^d_{yy}}{2}\right)^2 + (\sigma^d_{xy})^2} \tag{2.53}$$

$$f_{xz} = \frac{1}{2}(\sigma^d_{xx} + \sigma^d_{zz}) + \sqrt{\left(\frac{\sigma^d_{xx} - \sigma^d_{zz}}{2}\right)^2 + (\sigma^d_{xz})^2} \tag{2.54}$$

$$f_{yz} = \frac{1}{2}(\sigma^d_{yy} + \sigma^d_{zz}) + \sqrt{\left(\frac{\sigma^d_{yy} - \sigma^d_{zz}}{2}\right)^2 + (\sigma^d_{yz})^2} \tag{2.55}$$

Note that equation (2.52) is identical to equation (2.51) whenever $f_{xy} > f_{xz}$ and $f_{xy} > f_{yz}$.

This fracture model may be improved later. Additional discussion pertaining to fracture is contained in Section II-8 of Reference 1.

5. Initial and Boundary Conditions

The K3 activity space is a region whose left and right, bottom and top, back and front sides are parallel to the yz, xz, xy coordinate planes, respectively. The finite difference mesh, to be discussed in a later section, is imposed upon this region. All properties of the material within this region must be specified as initial conditions to the computational procedure. Many of these conditions are specified via the equation of state. The required initial input parameters for a material are

ρ - density

T or P - temperature or pressure

V_i - velocities

σ^d_{ij} - stress deviators

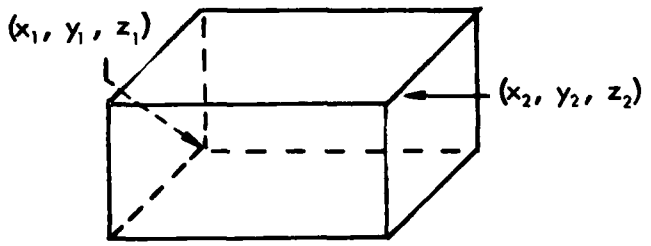
along with some geometrical parameters that describe the shape of the material. Usually the initial conditions on the stress deviators are zero.

Material is inserted into the activity space by defining a closed shape around the material. Several analytic forms corresponding to various shapes have been put into K3 to aid the user when inserting material into the mesh. The geometrical parameters in these forms must be specified whenever they are used. Figure II-1 shows the five different shapes currently available in K3, along with the associated geometric parameters that are required.

1. Special box (edges parallel to x, y, z axes)

Required Parameters

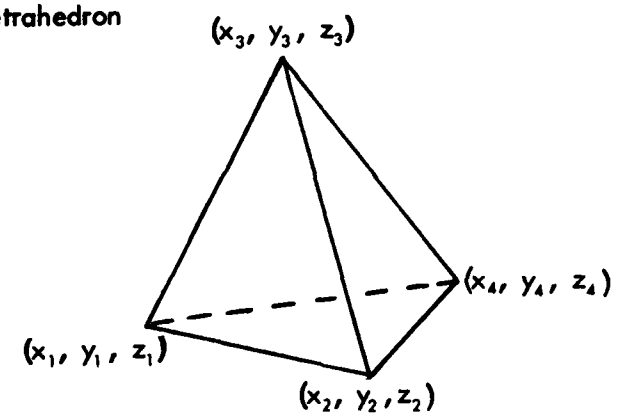
$x_1, y_1, z_1, x_2, y_2, z_2$



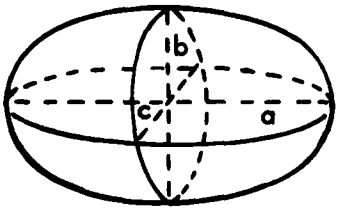
2. Tetrahedron

$x_1, y_1, z_1, x_2, y_2, z_2$

$x_3, y_3, z_3, x_4, y_4, z_4$



3. Ellipsoid



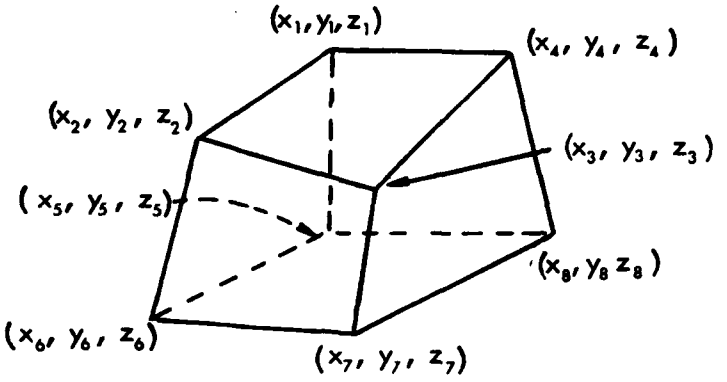
(x_c, y_c, z_c) -center

a, b, c semi major axes along x, y, z axes

FIGURE II-1

GEOMETRICAL SHAPES AVAILABLE FOR MATERIAL REPRESENTATION

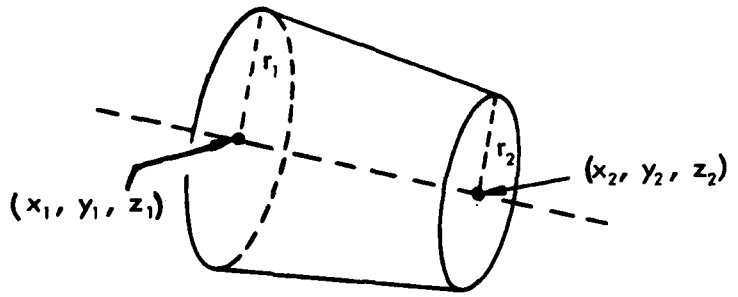
4. General solid with six faces



Required Parameters

$x_1, y_1, z_1, x_2, y_2, z_2$
x_3, y_3, z_3 x_4, y_4, z_4
$x_5, y_5, z_5, x_6, y_6, z_6$
$x_7, y_7, z_7, x_8, y_8, z_8$

5. Conical Frustrum



$x_1, y_1, z_1, x_2, y_2, z_2$
r, r_2-radii

FIGURE II-1 (continued)

GEOMETRICAL SHAPES AVAILABLE FOR MATERIAL REPRESENTATION

New material regions can be inserted into the activity space by combinations of insertions and deletions of the shapes currently in K3. For example, insertion of a large cube followed by deletion of an ellipsoid contained within the cube will result in a new material region that may be useful. This capability permits the user to insert some new shapes easily.

The properties of a material must also be specified. The values of ρ, T, V_x, V_y and V_z are always required. Specification of the stress deviators is required whenever elastic effects are to be treated. Whenever the initial state is uniform over a given region in the material, only a single value of each parameter need be specified. Fits to these parameters may have to be supplied whenever these parameters are dependent on the x, y and z coordinates.

K3 has the capability to impose independent boundary conditions on the boundaries. Currently the following four options are available for each boundary:

- o Reflective boundary
- o Transmittive boundary - material can leave but not enter mesh
- o Transmittive boundary - material may leave or enter mesh
- o Transmittive boundary - material may leave or enter mesh except external boundary pressures can be defined by input

Special coding is usually required for the last option.

6. Energy and Momentum Accounting

The CSQ relations pertaining to energy in Section II-12 of Reference 1 were left intact. However, modifications to the momentum accounting relations were required as follows.

The components of momentum in the i^{th} coordinate direction are

$$H_i(t) = \int_U V_i(U)\rho(U)dU \tag{2.56}$$

where U is the computational mesh volume. Note that the component $H_z(t)$ has been added for the K3 computation.

The momentum lost or gained due to material crossing the mesh boundaries can be expressed as several terms at the outer boundaries. These relations are extensive and thus will be expressed in compact form.

Let

$$\begin{aligned} \Phi &= 1 \qquad \text{if } V_n > 0 \\ &= 0 \qquad \text{if } V_n < 0 \end{aligned} \tag{2.57}$$

and let A denote surface area. Here V_n is a normal velocity component to the surface A considered. Anchoring these conventions to the computation mesh considered, the following functions can be defined for $1 \le i \le 3$, $1 \le k \le 2$:

$$\begin{aligned} A_{i1} &= A_{left} \qquad \text{if } i = 1 \\ &= A_{bottom} \qquad \text{if } i = 2 \\ &= A_{back} \qquad \text{if } i = 3 \end{aligned} \tag{2.58}$$

$$\begin{aligned} A_{i2} &= A_{right} \qquad \text{if } i = 1 \\ &= A_{top} \qquad \text{if } i = 2 \\ &= A_{front} \qquad \text{if } i = 3 \end{aligned} \tag{2.59}$$

$$\Phi_{ik} = 1 \qquad \text{if } V_i > 0 \qquad \text{on } A_{ik}$$

$$= 0 \qquad \text{if } V_i < 0 \qquad \text{on } A_{ik} \tag{2.60}$$

The above conventions can be used to represent the momentum accounting relations compactly. The rate that the i direction momentum flows out of the mesh is, for $i \neq j$, $i \neq k$, $j \neq k$,

$$\dot{H}_{i\ out} = \int_{A_{i2}} V_i^2\, \rho\Phi_{i2} dA - \int_{A_{i1}} V_i^2\, \rho\Phi_{i1} dA$$

$$+ \int_{A_{j2}} V_i V_j \rho\Phi_{j2} dA - \int_{A_{k1}} V_i V_j \rho\Phi_{j1} dA$$

$$+ \int_{A_{k2}} V_i V_k \rho\Phi_{k2} dA - \int_{A_{k1}} V_i V_k \rho\Phi_{k1} dA \tag{2.61}$$

Similarly,

$$\dot{H}_{i\ in} = \int_{A_{i2}} V_i^2 \rho(\Phi_{i2} - 1) dA - \int_{A_{i1}} V_i^2 \rho(\Phi_{i1} - 1) dA$$

$$+ \int_{A_{j2}} V_i V_j (\Phi_{j2} - 1) dA - \int_{A_{j1}} V_i V_j (\Phi_{j1} - 1) dA$$

$$+ \int_{A_{k2}} V_i V_k (\Phi_{k2} - 1) - \int_{A_{k1}} V_i V_k (\Phi_{k1} - 1) dA \tag{2.62}$$

The net flows at time t are

$$H_{i\ out} = \int_{t_o}^{t} \dot{H}_{i\ out}\, dt \tag{2.63}$$

$$H_{i\ in} = \int_{t_o}^{t} \dot{H}_{i\ in}\, dt \tag{2.64}$$

The differences

$$H_{i\ Rest}(t) = H_i(t) - H_{i\ out}(t) + H_{i\ in}(t) \tag{2.65}$$

represent the contributions from all other effects.

B. NUMERICAL CONSIDERATIONS

1. Finite Difference Mesh

The finite difference mesh in K3 is defined in space and time. The spatial mesh is defined by the user while the time mesh is usually constructed by the program to fit the problem considered as the calculation proceeds. Typically, if the conditions are known at time t_ℓ, the finite difference algorithm provides the conditions at a slightly later time $t_{\ell+1}$. The time step is $\Delta t = t_{\ell+1} - t_\ell$ for this cycle. The next cycle would have another time step $\Delta t = t_{\ell+2} - t_{\ell+1}$. This process is continued until conditions are known for the time range of interest. Restrictions on the computed time step that pertain to algorithm stability are presented in Section B-3.

The K3 spatial mesh is imposed by the user on the activity space considered. All of this space is partitioned into a three dimensional grid by three sets of parallel planes. These mesh planes are always parallel to the xy or xz or yz coordinate planes. The solid boxes formed by the intersections of these mesh planes are termed the cells. Since K3 is Eulerian in nature, the mesh planes remain fixed throughout the entire calculation. They are temporarily distorted during the Lagrangian phase of a given cycle, but are returned to their original position for the next cycle.

Material and energy flow through the fixed mesh and perhaps into and out of the mesh at the outer boundaries. Boundary condition computations determine whether flow is permitted across the outer edges. The mesh should be defined sufficiently large so that any material flow of significance is contained within it.

Let I_{max}, J_{max} and K_{max} denote the number of mesh increments in the x, y and z directions, respectively, as determined by the planes that partition the activity space. Then $I_{max}\ J_{max}\ K_{max}$ is the total number of cells in the mesh. The total number of grid points (x_i, y_j, z_k) is $I_{pax}\ J_{pax}\ K_{pax}$, where

$I_{pax} = I_{max} + 1$, $J_{pax} = J_{max} + 1$ and $K_{pax} = K_{max} + 1$. A simplified schematic of a K3 mesh is shown in Figure II-2. In this figure $I_{max} = 6$, $J_{max} = 6$ and $K_{max} = 4$; thus there are 144 cells and 245 grid points.

It is apparent from Figure II-2 that each cell can be uniquely identified as $\{ijk\}$. A typical cell is shown in Figure II-3. Note the center of the cell with coordinates $(x_{i + 1/2}, y_{j + 1/2}, z_{k + 1/2})$ and the center points of the six cell faces. The volume U_{ijk} of the cell is

$$U_{ijk} = (x_{i+1} - x_i)(y_{j+1} - y_j)(z_{k+1} - z_k) \tag{2.66}$$

The cells in the mesh need not all be of the same size. Variable spatial zoning in the coordinate directions can be used to obtain variable cell size in the mesh. Some variable computational zoning relations are presented in Reference 1. These are available in K3GEN.

Material zoning and rezoning for the CSQ finite difference mesh is discussed in Section III-3 of Reference 1. In K3 material rezoning was not considered. However, material zoning was implemented in K3GEN. Since the CSQ zoning presentations in Section III-3 of Reference 1 can readily be extended to three dimensions, no further discussion on K3 material zoning is given here.

2. Finite Difference Relations

The finite difference forms in K3 are based on the physical relations required for three dimensional flow. The K3 algorithm containing the difference forms is very similar in structure and procedure to the CSQ finite difference algorithm. At the beginning of each computational cycle the problem conditions are assumed known. The difference equations and associated

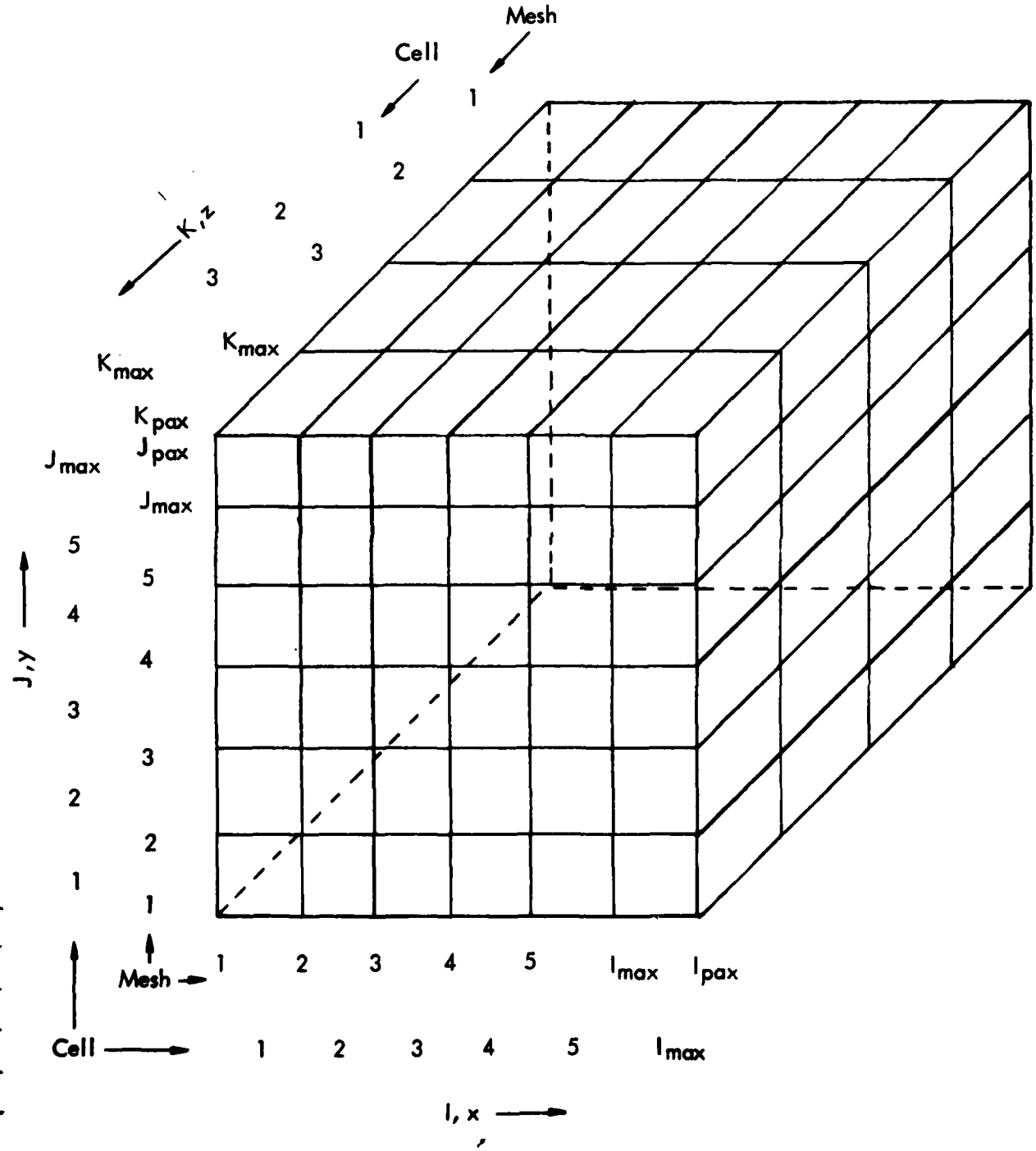


FIGURE II-2
SCHEMATIC OF K3 SPATIAL MESH

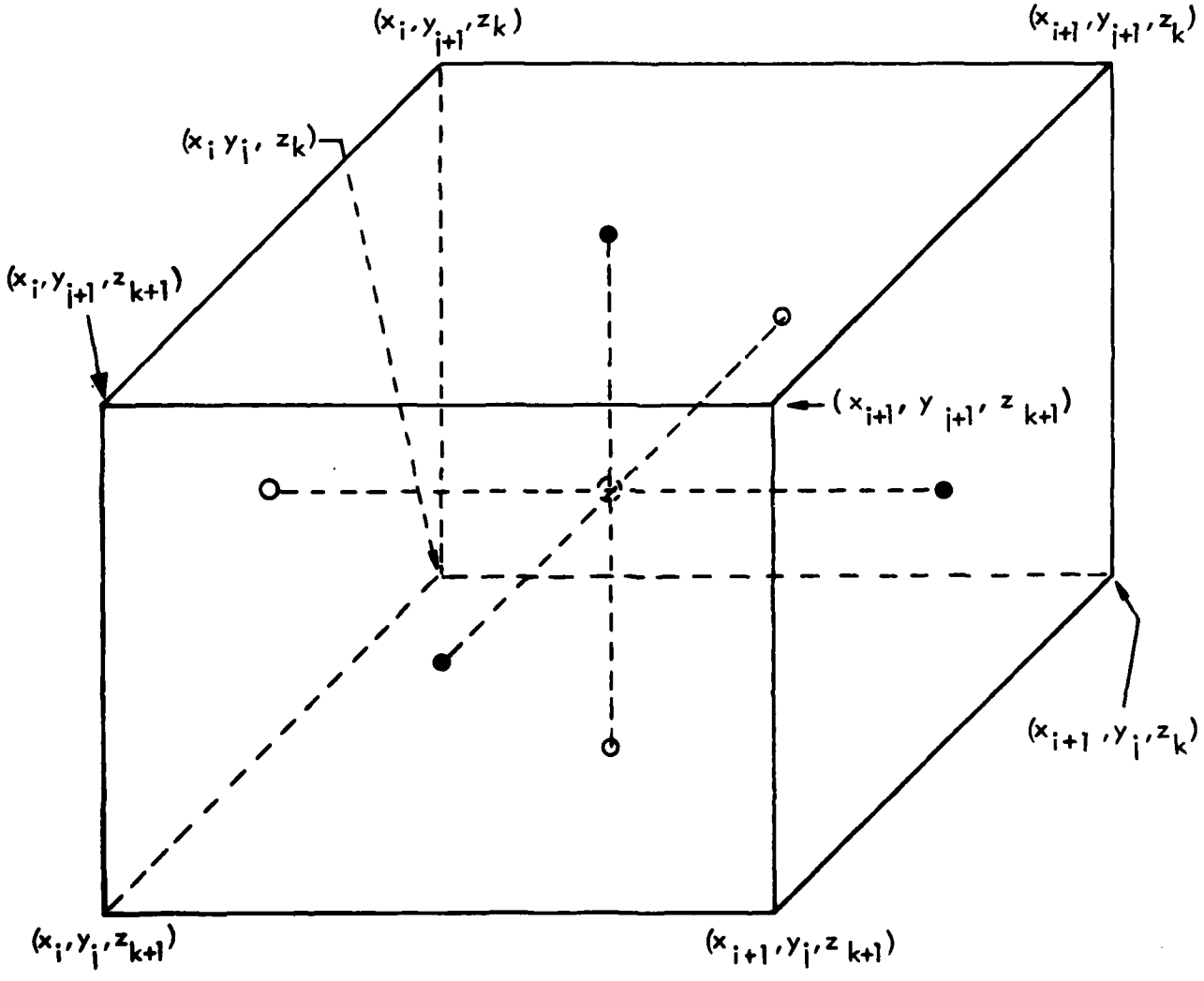


FIGURE II-3
THREE DIMENSIONAL CELL (i, j k)

boundary conditions determine the conditions at a slightly later time in the current Lagrangian coordinate system. The spatial mesh becomes distorted during this portion of the computational cycle. The Eulerian part of the cycle then redefines the distorted spatial mesh to its original position. Other computations may then be performed to complete the cycle.

The K3 finite difference algorithm requires three spatial indices i, j, k and one time index ℓ. These indices can be used to indicate where quantities are evaluated relative to the space time algorithm. Assuming that the indices i, j and k are used per the spatial mesh as indicated in Section B1, the velocities can be written

$$V_x(i, j + 1/2, k + 1/2, \ell + 1/2)$$

$$V_y(i + i/2, j, k + 1/2, \ell + 1/2)$$

$$V_z(i + 1/2, j + 1/2, k, \ell + 1/2)$$

to indicate that they are evaluated at the left, bottom and back faces of cell $\{ijk\}$ at time $t_{\ell + 1/2} = \frac{1}{2}(t_\ell + t_{\ell+1})$. Similarly, cell centered quantities such as pressure P can be written

$$P(i + 1/2, j + 1/2, k + 1/2, \ell)$$

to indicate they are evaluated at the center of cell $\{ijk\}$ at time t_ℓ.

The three dimensional finite difference relations for the Lagrangian portion of K3 are extensive and will not be presented here. Since the three dimensional counterpart of the CSQ difference forms can frequently be easily deduced, the user can consult Section IV of Reference 1 to determine information about the K3 difference forms.

The Eulerian section of K3 rezones the results of the Lagrangian portion of each cycle so that the mesh overlays its position at the start of the cycle. This requires the movement of mass, energy and other physical quantities between the various cells. In CSQ a geometrical interpretation coupled with conservation rules is used. The approach is one-diminsional in nature with necessary two-dimensional corrections. Further, one dimensional rezoning is used for each of the i and j strips in the CSQ mesh. Biasing due to this approach is minimized by interchanging the i-j order on alternate cycles.

The one-dimensional approach in CSQ was retained in K3. Extensions and modifications had to be made to ensure that the appropriate corrections were made and biasing kept miminal. Note that on each cycle there are three one-dimensional passes, since there are three independent coordinate directions.

The order of the i, j and k columns in K3 relative to the time cycles is as follows:

Cycle →	0	1	2	3	4	5	.	.	.
	j	i	k	j	i	k	.	.	.
Column →	k	j	i	k	j	i	.	.	.
Order	i	k	j	i	k	j	.	.	.

Note that the column order is repeated every three cycles. It is believed that permuting the column order in K3 as shown here will minimize biasing due to the one-dimensional column approach used.

The Eulerian finite difference relations in Section V of Reference 1 are essentially unchanged for K3, since they are one dimensional in character. Thus, they are not presented here. Also, the steps listed in subroutine EULER for the alternating direction method are valid for K3 provided "alternating" and "strip" are replaced by "permuting" and "column", respectively.

3. Time Step Controls

The time step for the K3 finite difference scheme must be selected so that the entire computation remains stable. This is accomplished by selecting the time step Δt_{cs} so that for any active cell ijk

$$\Delta t_{cs} \leq \text{Min} \left[\frac{x_{i+1} - x_i}{\phi_{ijk} + .5|V_{xi} + V_{xi+1}|} , \frac{y_{j+1} - y_j}{\psi_{ijk} + .5|V_{yj} + V_{yj+1}|} , \right.$$

$$\left. \frac{z_{k+1} - z_k}{\eta_{ijk} + .5|V_{zk} + V_{zk+1}|} \right] \tag{2.67}$$

where

$$\phi_{ijk} = \varepsilon C_s \quad \text{if} \quad \Delta V_x \geq 0$$

$$= A + \sqrt{A^2 + \varepsilon^2 C_s^2} \quad \text{if } \Delta V_x < 0 \tag{2.68}$$

$$\psi_{ijk} = \varepsilon C_s \quad \text{if} \quad \Delta V_y \geq 0$$

$$= B + \sqrt{B^2 + \varepsilon^2 C_s^2} \quad \text{if } \Delta V_y < 0 \tag{2.69}$$

$$\eta_{ijk} = \varepsilon C_s \quad \text{if} \quad \Delta V_z \geq 0$$

$$= C + \sqrt{C^2 + \varepsilon^2 C_s^2} \quad \text{if } \Delta V_z < 0 \tag{2.70}$$

$$A = B_{\ell}C_s - B_q\Delta V_x \tag{2.71}$$

$$B = B_{\ell}C_s - B_q\Delta V_y \tag{2.72}$$

$$C = B_{\ell}C_s - B_q\Delta V_z \tag{2.73}$$

$$\varepsilon = \text{Max}\left[\frac{3(1 - \nu_{\ell})}{1 + \nu_{\ell}}\right] \tag{2.74}$$

where ℓ is the material index and ν_{ℓ} is Poisson's ratio of the ℓth material.

Let $\tilde{\Delta t}_{cs}$ be the smallest value that results from application of the right side of (2.67). The Courant form of the time step is

$$\Delta t_{cs} = f_1\tilde{\Delta t}_{cs} \tag{2.75}$$

where $0<f_1\leq 1$. The default value for f_1 in K3 is 0.6.

The rate of increase of Δt between cycles in K3 is controlled as in CSQ. If Δt^1 is the Δt of the last cycle, then Δt_{inc} is defined as

$$\Delta t_{inc} = f_2\Delta t^1 \tag{2.76}$$

The default value of f_2 is 1.068000433. K3GEN further reduces the value of Δt for the first cycle of a computation.

Whenever the time step is to remain within a certain range, the input parameters Δt_{max} and Δt_{min} are used to provide the upper and lower bounds. The final value of Δt in this instance is

$$\Delta t = \max [\Delta t_{min}, \text{Min}(\Delta t_{cs}, \Delta t_{inc}, \Delta t_{max}, \Delta t_{rad})] \tag{2.77}$$

Here Δt_{rad} is idle in K3 since the radiation option in CSQ was left intact.

III PROGRAMMING CONSIDERATIONS

A. RESTART AND PLOT TAPE FORMATS

The following is the structure used by K3 input/output units 1, 2, and 3; K3GEN units 1 and 5; and K3PLT input units 1 through 5. All data are unformatted (binary). The general file layout is shown in Figure III-1 below, followed by a description of the individual records in each record block.

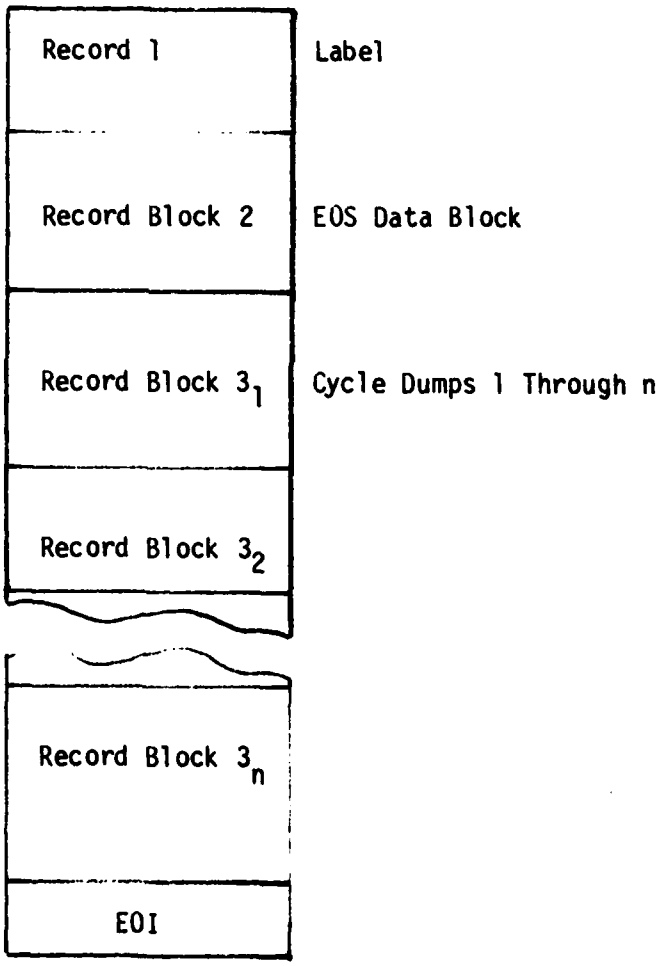


Figure III-1. Restart/Plot Tape File Structure

Record 1 - Problem Identification Format (10A10)

(LAB(ℓ), ℓ = 1, 10)

Record Block 2 - EOS Data Block

Record 2_a (ND(ℓ), ℓ = 1, 6)

Record 2_b (A(ℓ), ℓ = 1, ND(1))

Record 2_c (K(ℓ), ℓ = 1, ND(2))

Record 2_d (A(ℓ), ℓ = 1, ND(3))

There are ND(4) of the following record [ND(4)$\geq$ 0]

Record 2_e (A(ℓ), ℓ = 1, ND(5))

Following record is present only if ND(6) = 1

Record 2_f (A(ℓ), ℓ = 1, 8267)

where ND(1) $\leq$ 10

ND(2) = 142

ND(3) = 7321

$0 \leq$ ND(4) $\leq$ 10

ND(5) = 6851

ND(6) = 0 or 1

Record Block 3 - Cycle Dump

Record 3_a NI, NF, (NARRX(ℓ), ℓ = 1, NI), (ARRX(ℓ), ℓ = 1, NF)

where NI = 112

NF = 1168

For the following record, IMAX = NARRX(13)

JMAX = NARRX(14)

KMAX = NARRX(104)

Record 3_b ((VXL(ℓ,m), ℓ = 1, JMAX), m = 1, KMAX),

((VYL(ℓ,m), ℓ = 1, IMAX), m = 1, KMAX),

((VZL(ℓ,m), ℓ = 1, IMAX), m = 1, JMAX)

Record 3_c There are KMAX*IMAX records of the form

(STORE(ℓ), ℓ = 1, JNVAR)

where JNVAR = NARRX(20). Each record is an ik-column, i.e., all cell variables for a column of cells $1 \leq j \leq$ JMAX.

Following the last column record there is the start of the next cycle dump (Record 3_a) or an end-of-file.

B. CELL VARIABLES AND STORAGE ARRAYS

A set of variables must be retained for each cell in the K3 mesh. The storage variables are defined in such a way that only those variables required for the problem at hand are retained. Table III-1 lists the variables that may be associated with each cell. The basic number of variables required is ten and may range up to 40. To facilitate the storage of a variable number of cell variables, an array called LK(ℓ) is defined which contains the relative location of each cell variable associated with a particular cell. An ℓ value is associated with each cell variable, e.g., ℓ = 1 is pressure, ℓ = 2 is temperature, etc. LKℓ and LK(ℓ) are equivalenced in the coding of K3 for ease of computations. Example: If there are NVAR variables retained per cell and all data are stored sequentially in an array called STORE, it follows that the temperature of the third cell is located at STORE(2*NVAR+LK2).

Since there are NVAR*IMAX*JMAX*KMAX cell variables, it would be impractical to store all of this information in central memory except for very small values of IMAX, etc. or very large computers. Thus, cell variables are stored in ECS (or LCM) to the extent of available ECS, with excess information stored in Random Acess Mass Storage (disk). In ECS, the cell variables are arranged in terms of a index n given by

$$n_{ijk} = [(k-1)i_{max}]j_{max} + (i-1)j_{max} + j$$

where i, j, k are the indices of a particular cell. The variables for a given cell i, j, k are then located in ECS locations [(n-1)*NVAR+1] to [n*NVAR], assuming the cell variables are located in ECS and not on disk. If some, or all, cell variables are located on disk, matters become more complicated. In this case, Random Mass Storage indices are required to locate the desired cell information on disk (all variables associated with any one cell comprise one record on disk). These indices are also stored in ECS. Thus, ECS must be partitioned to accommodate as many cell variables as possible and also the

TABLE III-1

Cell Storage Variables

Variable		ℓ	LK(ℓ) Value
P	(pressure)	1	1
T	(temperature)		
C_s	(sound speed)	3	*
U	(cell volume)	4	*
V_y	(y velocity, bottom of cell)	5	3
V_x	(x velocity, left of cell)	6	4
E.	(· specific energy)	7	5
M.	(· mass)	8	6
E_x	(x specific energy)	9	7
M_x	(x mass)	10	8
Φ_x	(x material volume fraction)	11	9
Φ_v	(void volume fraction)	12	*
λ_r	(mean free path)	13	*
σ^d_{xx}	(stress deviator)	14	*
σ^d_{xy}	(stress deviator)	15	*
σ^d_{yy}	(stress deviator)	16	*
HE variable 1		17	*
HE variable 2		18	*
reserved for code expansion		19	*
position for start of material arrays		20	*
V_z	(z velocity, back of cell)	21	**
σ^d_{xz}	(stress deviator)	22	*
σ^d_{yz}	(stress deviator)	23	*
σ^d_{zz}	(stress deviator)	24	*
reserved for code expansion		25	*

*Indicates variables retained only if required for problem under consideration. Actual values for a given computation can be determined from the listing of the NARRX array output in K3GEN and K3 runs. Note that LK(1) = NARRX(55), etc.

† $\tilde{\Phi}_2$ =STORE(JVAR+LK20+1)
E_2 =STORE(JVAR+LK20+2)
M_2 =STORE(JVAR+LK20+3)
$\tilde{\Phi}_3$ =STORE(JVAR+LK20+4)
.
.
.
M_{N-1} =STORE(JVAR+LK20+[N-2])
JVAR ={(cell number - 1)NVAR}

** V_z is required in every three dimensional problem. Also, LK21=LK20+3(N-1)+1 where N is the number of materials.

indices to Random Mass Storage records for the cell variables that must be stored on disk. The partitioning is done by an alternate entry to Subroutine GETPUT, and is based upon the amount of available ECS, information supplied by Subroutine MEM. It is advantageous to try to fit all of the cell variables into ECS by setting the size of ECS as large as possible and/or scaling down the number of cells, since using disk results in a longer running program (the ratio of wall clock time to central processor time increases considerably).

The actual location of cell variables, either on disk or in ECS, is transparent to the program and user (except where run time is increased) since the storing and fetching of these variables is handled by one routine, GETPUT. This routine works with one "strip" at a time where a strip is all of the variables associated with a column or row of cells, i.e., all cells where i and k are constant and j varies from 1 to j_{max}, or i and j are constant and k varies from 1 to k_{max}, etc. To handle the cell variables associated with a strip a series of STORE arrays (STORE, STOREL, STORER, etc), dimensioned NVAR* max (i_{max}, j_{max}, k_{max}), are defined in K3GEN and K3. GETPUT will fetch a strip from ECS or disk to one of the STORE arrays, the main routines will process and modify information where required, and then call GETPUT to store the information back to ECS or disk before moving on to the next strip.

Additional arrays are required to hold the cell location and size information (X, Y, Z, ΔX, ΔY, ΔZ) and also the velocities at the top, right, and front of the mesh (VYL, VXL, VZL). These latter arrays are also stored in ECS. At present the dimensions of the arrays are set to accommodate up to 80 cells in each X, Y or Z direction. If these are increased, variable NECSL in K3GEN must be redefined to indicate the new length of common /VEL/, and KMAXM, JMAXM, IMAXM, also in K3GEN, must be reset to the maximum number of cells allowed.

Two arrays, NARRX and ARRX, are located at the beginning of blank common in K3GEN and K3. These are user-accessible arrays with provisions made in K3 for changing any variable in either array by input cards in K3. Table III-2 lists the variables and their use (--- indicates an unused variable) in these two arrays.

TABLE III-2

Blank Common Variable List for K3

NARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
1		Number of Variables in ARRX Array Before Geometry Arrays (114 for present code)
2		First Location in ECS/LCM for Main Mesh Storage Arrays
3		---
4		---
5		Flag for Suppression of Thermal & Plasma Conduction 0 - Normal 1 - Suppress
6		HE Burn Flag (IBURNHE input variable) 0 - No Burn $\pm$ - Burn HE (Idle - not operational)
7		Current Number of Energy Flow Subcycles Allowed
8		Maximum Number of Energy Flow Subcycles Allowed
9		Energy Flow Cycle Number
10		---
11	I	Mesh Index
12	J	Mesh Index
13	IMAX	See Section II-B-1
14	JMAX	See Section II-B-1
15	IPAX	See Section II-B-1
16	JPAX	See Section II-B-1
17	IACT	See Section II-B-1
18	JACT	See Section II-B-1

NARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
19	NVAR	Number of cell variables
20	JNVAR	JMAX*NVAR
21	NORAD	Energy Flow Switch 0 - No Energy Flow Computation 1 - Energy Flow Computation on (Idle - not operational)
22	NVOID	Cell Void Flag 0 - Retain Cell Void Fractions 1 - Do Not Retain
23	NEXTV1	Print Variable Flag
24	NEXTV2	Print Variable Flag
25	NEXTV3	Print Variable Flag
26	ICYCLE	Hydro Cycle Number
27	ICOUNTS	Short Edit Number
28	ICOUNTL	Long Edit Number
29	NDUMP	Restart Dump Number
30	MDUMP	Plot Dump Number
31	ICYCLES	End of Problem Cycle
32	NEXTP	Flag for Special Edit
33	NDTCS	Cell Number Controlling Δt_{cs}
34	NDTCSN	Same as 33 for Next Cycle
35	NDTRAD	Cell Number Controlling Δt_{rad} (Idle)
36	NDTRADN	Same as 35 for Next Cycle (Idle)
37	IGM	Geometry Flag δ 0 = Rectangular 1 = Cylindrical (Idle - not operational)

NARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
38	NUMMT	Number of Material
39	NUMMX	Number of X Materials (NUMMT-1)
40	KAB(1)	KAB(1) to KAB(10) are Hollerith Fields with Problem Identification
41	KAB(2)	
42	KAB(3)	
43	KAB(4)	
44	KAB(5)	
45	KAB(6)	
46	KAB(7)	
47	KAB(8)	
48	KAB(9)	Current Date
49	KAB(10)	Current Clock Time
50	KLAB(1)	KLAB(1) to KLAB(4) are Hollerith Fields with Edit Titles
51	KLAB(2)	
52	KLAB(3)	
53	KLAB(4)	
54	KPLOT	Short Edit Line Printer Plot Flag 0 - No Plot 1 - Material Plot Only -1 - Momentum Plot Only 2 - For Both Plots (Normal)

NARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
55	LK1,LK(1)	LK1 to LK25, See Table III-1
56	LK2,LK(2)	
57	LK3,LK(3)	
58	LK4,LK(4)	
59	LK5,LK(5)	
60	LK6,LK(6)	
61	LK7,LK(7)	
62	LK8,LK(8)	
63	LK9,LK(9)	
64	LK10,LK(10)	
65	LK11,LK(11)	
66	LK12,LK(12)	
67	LK13,LK(13)	
68	LK14,LK(14)	
69	LK15,LK(15)	
70	LK16,LK(16)	
71	LK17,LK(17)	
72	LK18,LK(18)	
73	LK19,LK(19)	
74	LK20,LK(20)	
75	LK21,LK(21)	
76	LK22,LK(22)	
77	LK23,LK(23)	
78	LK24,LK(24)	
79	LK25,LK(25)	

NARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
80	NELEP	Elastic Plastic Switch 0 - No EP Calculation 1 - EP Calculation on
81	NPORFG(1)	Distended Material Switch for Material 1 = 0 not distended = 1 can be distended
82	NPORFG(2)	Same as NPORFG(1) except for material indicated
83	NPORFG(3)	
84	NPORFG(4)	
85	NPORFG(5)	
86	NPORFG(6)	
87	NPORFG(7)	
88	NPORFG(8)	
89	NPORFG(9)	
90	NPORFG(10)	
91	MMMM(1)	Tracer Particle Storage Index (Idle - not operational)
92	MMMM(2)	Tracer Particle Storage Index (Idle - not operational)
93	MMMM(3)	Maximum I Mesh Size Possible (Size of Dimension Statements, 80 for Present Code)
94	MMMM(4)	Same as 93 Except for J Mesh
95	MMMM(5)	I Mesh Index for Activation Calculation
96	MMMM(6)	J Mesh Index for Activation Calculation
97	MMMM(7)	Current Number of Energy Flow Subcycles
98	MMMM(8)	---
99	MMMM(9)	---
100	MMMM(10)	---

NARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
101	K3	Mesh Index
102	KMAX	See Section (II-B-1)
103	KACT3	See Section (II-B-1)
104	KPAX	See Section (II-B-1)
105	LKA1	Auxillary Variable with Value One
106	LKA2	Auxillary Variable with Value Two
107	LKA3	Auxillary Variable with Value Three
108	LKA4	Auxillary Variable with Value Four
109	IJNVAR	IMAX*JMAX*NVAR
110	MMMM1(1)	Available LCM for Cell Storage Set by GETPUT
111	MMMM1(2)	
112	MMMM1(3)	Size of Common /VEL/

ARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
1		Minimum Velocity for Cell Activation
2		Minimum Fractional Temperature Difference for Cell Activation
3		Temperature Convergence Factor for Energy Balance Iterations
4		---
5		---
6		---
7		---
8		---
9		---
10		Flag to Suppress Writing of Global Quantities on History Tape 55. = 0 Write Global Quantities = 1 Do Not Write
11		Temperature Lower Limit for EOS Iterations
12		Flag for Viscosity Form. If>0 Use Q in Compression Only. = 0 Use Normal Q in Both Expansion and Compression. < 0 Use Normal Q in Compression and Linear Term in Expansion
13		Temperature Iteration Limit Factor
14		---
15		---
16		---

ARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
17		---
18		---
19		---
20	TEMPBG	Temperature Assigned to Void Cell if NORAD = 0
21		---
22		---
23		---
24		---
25		---
26		Factor in Energy Flow Time Step Control
27		Factor in Opacity Average
28		Factor in Energy Flow Time Step Control
29		Factor in Opacity Average
30	TMASS	Total Mass in Mesh
31	TMASSD	Total Dot Mass in Mesh
32	TMASSX	Total X Mass in Mesh
33	TIME	t = Problem Time
34	DT	Δt
35	DTH	$\Delta t'$
36	DTOLD	Δt of Last Cycle
37	DTCS	Δt_{cs}
38	DTCSN	Δt_{cs} for Next Cycle
39	DTRAD	Δt_{rad}

ARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
40	DTRADN	Δt_{rad} for Next Cycle
41	DTMAX	Δt_{max}
42	DTMIN	Δt_{min}
43	FRACDT	f_1
44	DTINCR	f_2
45	BQ	B_q
46	BL	B_ℓ
47	QCS	$C_{i_{ref}}$
48	QGAM	δ
49	VCUT	Cut Off Momentum for Short Edit Momentum Plots
50	ETOT	$\mathcal{E}_{initial} + S(t)$ (see Eqs. (2.106)(2.107) in Ref. 1)
51	HUP	$H_y(t)$
52	HRAD	$H_x(t)$
53	HFOR	$H_z(t)$
54	ERADIN	Radiation Energy Into Mesh
55	ERADOUT	Radiation Energy Out of Mesh
56	EINTIN	Internal Energy Into Mesh
57	EINTOUT	Internal Energy Out of Mesh
58	EKIN	Kinetic Energy Into Mesh
59	EKOUT	Kinetic Energy Out of Mesh
60	HUPIN	$H_y(t)$ Into Mesh
61	HRADIN	$H_x(t)$ Into Mesh
62	HUPOUT	$H_y(t)$ Out of Mesh

ARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
63	HRADOUT	$H_x(t)$ Out of Mesh
64	HFORIN	$H_z(t)$ Into Mesh
65	HFOROUT	$H_z(t)$ Out of Mesh
66	AMDIN	Dot Mass Flow Into Mesh
67	AMDOUT	Dot Mass Flow Out of Mesh
68	AMXIN	X Mass Flow Into Mesh
69	AMXOUT	X Mass Flow Out of Mesh
70	BSWTOP	Hydro Boundary Condition Option (Input Parameters)
71	BSWSID	Same as 70
72	BSWBOT	Same as 70
73	BSWINS	Same as 70
74	BSWFOR	Same as 70
75	BSWBAC	Same as 70
76	RADTOP	Energy Flow Boundary Condition Option (Input Parameter)
77	RADSID	Same as 76
78	RADBOT	Same as 76
79	RADINS	Same as 76
80	RADFOR	Same as 76
81	RADBAC	Same as 76
82	TSTOP	Current Problem Stop Time
83	GMINES	γ_{min}
84	GMAXES	γ_{max}
85	BURNP1	D/N - HE Burn Parameter
86	BURNP2	HE Predetonation Pressure

ARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
87	TSQUEN	Total Energy from Sources
88	PFR114	Parameter Used for Extrapolation of Boundary Pressures
89	BWORK	
90	RADK1	$4\ \sigma_s/c$
91	RADK2	$4\ \sigma_s/(3c)$
92	RADK3	$16\ \sigma_s/(3c)$
93	RADK4	$16\ \sigma_s/c$
94	RADK5	$\sigma_s/6$
95	RADK6	$\sigma_s/16$
96	RADK7	$\sigma_s/12$
97	RADK8	σ_s
98	RADK9	2/3
99	PIE	π (= 3.1415926..)
100	TWOPIE	2π
101	AMINM	Round Off Test for Empty Cell
102	DVOLVM	Cut Off Test Parameter for Kinetic Energy Corrector
103	EVOLCK	Maximum Relative Charge in Volume Allowed in Energy Balance
104	VCHECK	Smallest Allowed Velocity
105	VOLCK	Round Off Test Parameter for Volume Checks
106	RADAVS	Minimum Fractional Difference Between Adjacent Zone Temperatures to Compute Boundary Mean Free Path Values. If 0 - Always Use Cell Center Values
107	EMPTY	Scale Factor for Kinetic Energy Corrector (Normally 1)

ARRX	Other Names	Purpose, Quantity, Section or Equation of Definition
108	EARRX(1)	
109	EARRX(2)	
110	EARRX(3)	Extra Array Not Used in Current Coding
111	EARRX(4)	
112	EARRX(5)	
113	EARRX(6)	
114	EARRX(7)	

IV USER'S GUIDE

A. CONTROL CARDS FOR K3 PROGRAMS

The run sequence for a K3 calculation begins with PREK3. This program generates the COMDECKs necessary for compilation of K3GEN, K3, and K3PLT. The procedure used in the following examples of control card setup was to punch the COMDECKs, then physically insert the punched cards in the proper place in the K3GEN, etc., job decks. This procedure can certainly be modified to suit the needs or desires of individual users, limited only by the capabilities of the UPDATE program.

1. PREK3

```
Job card
ATTACH, A, K3.
UPDATE (P = A, C = PREK3, Q)
RETURN, A.
FTN (I = PREK3, L = 0)
RETURN, PREK3
LGO.
REWIND, DKCSQ.
COPYCF (DKCSQ, PUNCH)          Punch deck for K3GEN, K3, and K3PLT.
REWIND, DKCSQ.                 IOUT input variable set to 1 to
COPYCF (DKCSQ, PUNCH)          direct output to file DKCSQ.
REWIND, DKCSQ.
COPYCF (DKCSQ, PUNCH)
EXIT.
7/8/9
*C PRECSQ
7/8/9
- data card for PREK3 -
7/8/9
6/7/8/9
```

2. K3GEN

```
Job card
ATTACH (OLDPL, K3)
UPDATE (P, Q)
RETURN, OLDPL.
FTN (I, LCM = I, L = 0)
RETURN, COMPILE.
REQUEST, TAPE1, *PF.
LGO (PL = 50000)
CATALOG (TAPE1, RESTART)
EXIT.
7/8/9
*AF INPUT, YANK$$$
- COMDECKs created by PREK3 -
*C CSQGEN
7/8/9
- data cards for K3GEN -
7/8/9
6/7/8/9
```

3. K3

```
Job card
ATTACH (OLDPL, K3)
UPDATE (P, Q)
RETURN, OLDPL.
FTN (I, LCM = I, L = 0)
RETURN, COMPILE.
ATTACH (TAPE1, RESTART)
STAGE (TAPE2, POST)
LDSET (PRESET = ZERO)
LGO (PL = 50000)
EXIT.
```

3. K3 (continued)

```
7/8/9
*AF INPUT, YANK$$$
- COMDECKs created by PREK3 -
*C CSQ, EP
7/8/9
- data cards for K3 -
7/8/9
6/7/8/9
```

Note the compilation of the EP deck which contains the elastic-plastic routines. This deck may or may not be required depending upon the problem being run. Other decks which may be compiled such as the History package, Tracer package, etc., are not operational in the main K3 code.

4. K3PLT

```
Job card
ATTACH (OLDPL, K3)
UPDATE (P, Q, R)
REWIND, COMPILE.
FTN (LCM = I, I, L = 0)
UPDATE (F, P, C = SCORS, R)
REWIND, SCORS.
FTN (I = SCORS, L = 0, B = XLIB, LCM = I)
RETURN, SCORS, COMPILE, OLDPL.
REWIND, XLIB.
LIBEDT.
RETURN, XLIB.
ATTACH (ARCLIB, ARCLIB, ID = PRDLIB)
LIBRARY (SLIB, ARCLIB)
LDSET (PRESET = ZERO)
LGO.
EXIT.
```

4. K3PLT (continued)

```
7/8/9
*AF INPUT, YANK$$$
- COMDECKs from PREK3
*C CSQPLT
7/8/9
7/8/9
LIBRARY (SLIB, NEW = 4000)
ADD (*, XLIB)
FINISH
ENDRUN
7/8/9
7/8/9
6/7/8/9
```

The modified SCORS package of routines is put into a library in order to reduce the size of the executable program since only those routines required are loaded. No data cards are required since inputs are defined interactively, i.e., through keyboard inputs as the program executes.

B. INPUT INSTRUCTIONS

1. PREK3

The program PREK3 is a preprocessor for K3GEN, K3 and K3PLT. It generates COMDECKs for use by the UPDATE processor. It must be used to produce a program acceptable to the FTN compiler. Only one card is read by PREK3. Its format is as follows:

Card 1	Format (4I5)
(1-5)	IJMAX = largest mesh dimension (IMAX, JMAX or KMAX) $20 \leq$ IJMAX ≤ 80
(6-10)	NVAR = maximum number of variables per cell $10 \leq$ NVAR ≤ 40
(11-15)	MAXMS = maximum number of materials $2 \leq$ MAXMS ≤ 10
(6-20)	IOUT = output switch = 0, punched card output = 1, output to file DKSCQ

PREK3 also produces for user edification a listing of expected program memory requirements based upon the generated COMMON sizes. This listing has not been updated from CSQ requirements (K3 requires more space), hence should not be used to size programs until such time as it is modified.

2. K3GEN

The program K3GEN generates a new problem or rezones a previous K3 calculation. The following suggestions are included to aid the user. Their meaning will be clearer after going through the input instructions.

1. EOS and high explosive data should be checked with the test program CKEOS2.
2. ANEOS options -1, 0, and 1 should not be used with K3.
3. The cell activator works in increasing coordinate direction. Initial action should be in the lower left back corner of the mesh for calculational speed considerations.

4. During material zoning, subcell centers are tested to determine if a subcell is inside a zoning region.
5. If more than one material zoning region incloses a given spatial region, the first region data is used.
6. During a rezone any card inputs are processed before the old mesh data are considered. Because of 5 above, this means the card inputs will override old mesh data.
7. Cell centers are tested to determine if a cell is inside a region defined as high explosive.
8. ECS/LCM required is discussed in the text of report.
9. Only ANEOS options 3 and 4 and tabular EOS information should be used for porous materials.
10. During a rezone the ECS/LCM required is the larger of that required for the old or new mesh.
11. Rules for automatic determination of number of cell variables (NVAR) using data on card 4.

Start with NVAR = 10

Add 1	if NORAD > 0
Add 1	if NVOID = 0
Add 1	if CSSAVE = 1
Add 1	if VOLSAVE = 1
Add 6	if NELEP = 1
Add 2	if IBURNHE ≠ 0*
Add 3	for each material over two.

Tape Units K3GEN

1. Restart output tape (for K3)
2. Rezone input tape (from K3)*
5. Input tape from CHDCSQ† or internal storage during rezones*
12. EOS input tape for tabular data
72. Internal Storage
77. Random Mass Storage

* Not operational in present K3 code.

† Not tested

a. K3GEN Inputs

Card 1. Format (8A10)
80 Column Problem Identification
Any BCD Information

Card 2.	Format (1615)	
Variable 1.	NUMMT	Number of materials Cannot be larger than defined in PREK3 $2 \leq$ NUMMT ≤ 10.
Variable 2.	NREZONE	= 0 for generation of new problem > 0 for rezone of previous calculation with old EOS data using the NREZONEth dump on input unit 2.* < 0 for rezone of previous calculation with new EOS data (define as for new problem) using the |NREZONE|th dump on input unit 2. If NREZONE ≠ 0, insert Card Set R after Card Set 3 and see discussion at the end of this section.*
Variable 3.	NCHDZN	= 0 No input data from CHDCSQ = 1 To read input tape from CHDCSQ on tape Unit 5.† If NCHDZN = 1, then code sets NREZONE = 0 above; i.e., both features cannot be used at same time.
Variables	NEOS(KEOS) [KEOS = 1,...,NUMMT]	Equation of state number for material KEOS > 0 tabular (on Tape 12) = -1, -2,...,-NUMMT (ANEOS)

---

* Not operational in present K3 code.
† Not tested

Card Set 3. Analytic Equation-of-State Data

Any inputs for the ANEOS package go here. The formats are given in Appendix F of SLA-73-0477 (Reference 4) or section b, following this section. This is the same as Card Set 12 for CHART D. The identification variable in the ANEOS input format should agree with NEOS(KEOS) above. There is one set of cards for each unique NEOS(KEOS) < 0. They can be in any order.

Omit this card set if NREZONE > 0 on Card 1.

Card Set R.

If NREZONE ≠ 0 (Card 1) insert Card Set R here. See discussion at end of K3 instructions.

Card 4.	Format (1615)	
Variable 1. (1-5)	IGM	- geometry switch = 0 rectangular = 1 cylindrical (not operational)
Variable 2. (6-10)	NORAD	- energy flow switch = 0 no energy flow > 0 energy flow with NORAD the maximum number of subcycles allowed. (Not operational)
Variable 3. (11-15)	NVAR	= number of variables stored per cell. = 0 for code to calculate (normal) < 0 for code to calculate and then add -NVAR to result
Variable 4. (16-20)	NVOID	- void switch = 0 code carries cell void fractions (normal). Use 0 if any solids are present in mesh. = 1 code does not carry void fractions. Use 1 only if voids can never be present. (very high temperature, gases, etc.)

Variable 5. (21-25)	CSSAVE	- switch to save sound speed for printing = 0 do not save (normal) = 1 save sound speed
Variable 6. (26-30)	VOLSAVE	- switch to save cell volume for printing = 0 do not save (normal) = 1 save volume
Variable 7. (31-35)	NEXTV1	- print switch for nonstandard edit variable in 3rd from last edit column. printed variable is STORE(LK(NEXTV1)).* Default values are: 11 (Φ_x) if NORAD = 0 13 (λ_r) if NORAD ≠ 0
Variable 8. (36-40)	NEXTV2	- same as NEXTV1 except for second from last edit column. Default value is 7(E.).
Variable 9. (41-45)	NEXTV3	- same as NEXTV1 except for last edit column. Default value is 9(E_x).
Variable 10. (46-50)	NELEP	- switch for elastic plastic calculation = 0 EP calculation off = 1 EP calculation on
Variable 11. (51-55)	NPOROUS	- switch for porous material calculation = 0 porous material calculation off = 1 porous materials present-input card 7.
Variable 12. (56-60)	KATMOS	not used

*See Table III-1. Note if NEXTV1, 2, 3 = 14, 15, or 16 printed variable is σ_{xx}, σ_{xy}, σ_{yy} instead of σ^d_{xx}, σ^d_{xy}, σ^d_{yy}.

Variable 13. (61-65)	IBURNHE	= 0 if no high explosives are to be burned = 1 if high explosives are present (not operational). = -1 same as +1 except with predetonation print in CSQ (tells when cell starts burning). If IBURNEHE ≠ 0, see Card Set 11. (Not operational)
Variable 14. (66-70)	NTRACE	- switch for tracer particles = 0 no tracer particles = 1 input tracer particle data on Card Set 12. (Not operational) = -1 retain tracer positions from rezone data. (Not operational) = 2 retain tracer positions from rezone data and input more particle data on Card Set 12. (Not operational) LAST TWO OPTIONS APPLY ONLY TO REZONES (NREZONE ≠ 0 ON CARD 2).

Card 5.1	Format (8E10.3)	
Variable 1. (1-10)	XACT	- X position for active mesh if XACT $\leq$ XINSIDE (see below), code sets XACT = ∞
Variable 2. (11-20)	YACT	- Y position for active mesh if YACT $\leq$ YBOTTOM, code sets YACT = ∞
Variable 3. (21-30)	ZACT	- Z position for active mesh if ZACT $\leq$ ZBACK code sets ZACT = ∞

Variable 4. (31-40)	XINSIDE	= X(1)
Variable 5. (41-50)	YBOTTOM	= Y(1)
Variable 6. (51-60)	ZBACK	= Z(1)

Card 5.2	Format (8E10.3)	
Variable 1. (1-10)	BL	- linear viscosity coefficient
Variable 2. (11-20)	BQ	- quadratic viscosity coefficient If BL + BQ = 0, Code Sets BL = 0.1 and BQ = 2.0.
Variable 3. (21-30)	TIME	- initial problem time (normally 0). If a rezone is being done (NREZONE ≠ 0 on Card 2), input - 1. to retain time from rezone data.
Variable 4. (31-40)	TEMPBG	- background temperature (used as initial temperature in regions not included in Card Set 10.) Default value is 0.02567785ev (298°K).

Card 6.	Format (8F5.0, E10.3)	
Variable 1. (1-5)	BSWTOP	= mass boundary switch for top of mesh (options given below).
Variable 2. (6-10)	BSWBOT	= mass boundary switch for bottom of mesh
Variable 3. (11-15)	BSWSID	= mass boundary switch for right of mesh.

Variable 4. (16-20)	BSWINS	= mass boundary switch for left of mesh. (Not used if IGM = 1).
Variable 5. (21-25)	BSWBAC	= mass boundary switch for back of mesh.
Variable 6. (26-30)	BSWFOR	= mass boundary switch for front of mesh.
Variable 7. (31-35)	RADTOP	= radiation boundary switch for top of mesh.
Variable 8. (36-40)	RADBOT	= radiation boundary switch for bottom of mesh.
Variable 9. (41-45)	RADSID	= radiation boundary switch for right of mesh.
Variable 10. (46-50)	RADINS	= radiation boundary switch for left of mesh. (Not used if IGM = 1).
Variable 11. (51-55)	RADBAC	= radiation switch for back of mesh.
Variable 12. (56-60)	RADFOR	= radiation switch for front of mesh.
Variable 13. (61-65)	DTSTART	= fraction of normal time step to be used on cycle 1. If DTSTART $\leq$ 0, code sets DTSTART = 0.02.

BSW --- Options

0. Reflecting boundary
1. Transmittive boundary no mass allowed to enter mesh.
2. Same as 1 except mass can be drawn into the mesh.

RAD --- Options (Not Operational)

0. Reflecting boundary
1. Transmittive boundary with mass outside of mesh. Properties of external mass are interpolated from the properties inside mesh.
2. Same as Type 1 except external temperature is defined by input cards in K3. (See Card Set 14 in CSQ input, Reference 1).

3. Same as 2 except that external boundary pressure can be applied. Will require special coding in K3 subroutine PBTRP.	3. Transmittive boundary without mass outside of mesh. External temperature is defined by input cards in K3 (See Card Set 14 in CSQ input, Reference 1).

Card 7. Format (1015)

This set of cards is present only if NPOROUS = 1 on card 4. There is one input parameter for each material. I = 1, NUMMT.

Variable		
	NPORFG(KEOS) [KEOS=1,...,NUMMT]	= switch for porous material calculation for material KEOS. = 0 not porous = 1 material can be distended

---

Zoning the Problem

Each problem is zoned in two parts. There is a spatial card set (X, Y, Z) which defines the space fixed mesh. A material definition card set then follows to place the material in this mesh. Each card carries an identification field in columns 1 to 5 to aid in ordering the punch cards.

Identification	Concerns
40's	X spatial
50's	Y spatial
60's	Z spatial
70's	Insert material into mesh.
80's	Delete material (in relation to 70 cards).
90's	Material properties.

The numbers 40, 50, 60, 70 and 90 are only used as stop cards. Numbers 41, 93, etc., are employed to define information. As will be explained below, the order of the cards must be

41 - can be more than one.
40
51 - can be more than one.
50
61 - can be more than one.
60
71 to 74
79
81 to 84 - optional
89 - optional
91 to 94 - optional
90
70

} Repeat for each material package

NOTE: If present, Card Set G follows the 90 card. See discussion at end of K3GEN instructions.

Card Set 8. X Zoning

The zoning starts at the left of the mesh and works to the right. Note that XINSIDE = X(1) is defined on Card 5.1.

Card 8.1	Format (2I5, 4E10.3)
Variable 1. (1-5)	Integer 41
Variable 2. (6-10)	N = number of zones to be included with this card set.
Variable 3. (11-20)	DX = width of first zone (left side) in this region
Variable 4. (21-30)	X_t = total width of this region.
Variable 5. (31-40)	R = ratio of adjacent zone widths. (= $\Delta X_{i+1}/\Delta X_i$)

Variable 6. (41-50) DXL = width of last zone (right side) in this region.

Note: Define the variables by one of the following four options. Leave others blank.

Option	N	DX	X_t	R	DXL
1	✓	✓	✓		
2	✓	✓		✓	
3	✓		✓	✓	
4	✓ (N>2)	✓	✓		✓

R is not constant for Option 4

Keep repeating these cards until the entire X mesh is defined. When finished insert Card 8.2.

Card 8.2 Format (15) X zoning stop card

Variable 1. (1-5) Integer 40

Card Set 9.1 Y Zoning

The zoning starts at the bottom of the mesh and works upward. Note that YBOTTOM = Y(1) is defined on Card 5.1.

The information on the two forms of input cards is the same as Card Set 8 except that 51 and 50 are the identification numbers.

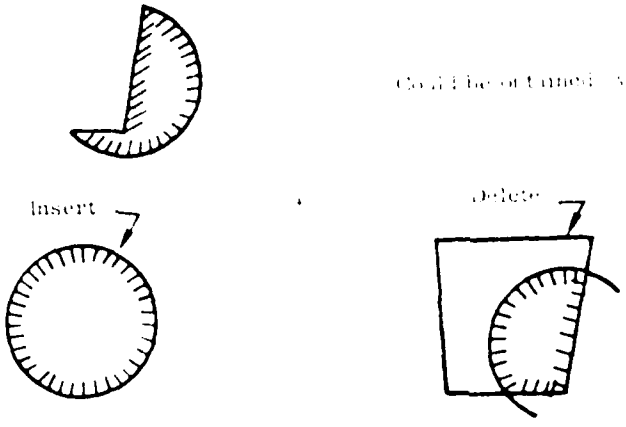
Card Set 9.2 Z Zoning

The zoning starts at the back of the mesh and works forward. Note that ZBACK = Z(1) is defined on Card 5.1.

The information on the two forms of input cards is the same as Card Set 8 except that 61 and 60 are the identification numbers.

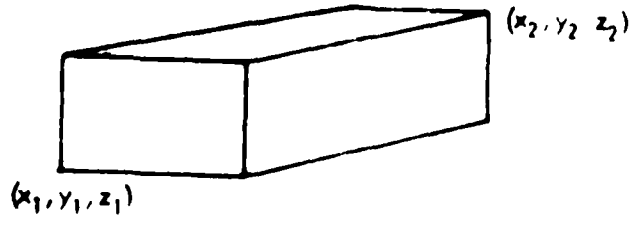
Material Zoning

In CSQ the material is placed in the space mesh by defining geometrical shapes in the X, Y plane and the properties of the material in this region. Shapes can be inserted and then partially deleted to obtain oddly configured material. For example the shape



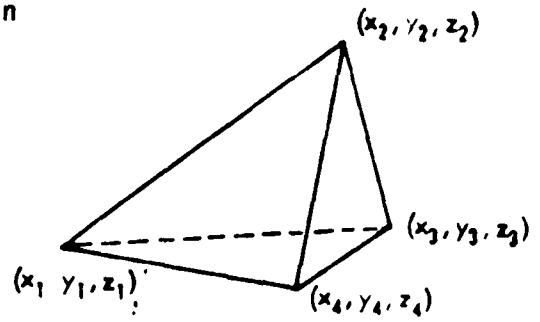
This method of material zoning for CSQ was generalized to three dimensions for K3. The shapes in K3 that can be inserted and then partially deleted to obtain irregular configured material are as follows.

1. Rectangular parallelepiped or box (edges parallel to x, y, z axis)



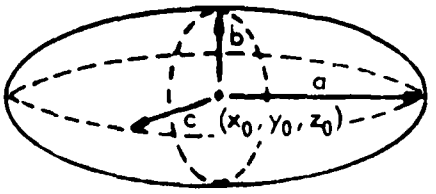
Code No.	79/89 Card	Variable		
71 - insert	1	X_1	4	X_2
81 - delete	2	Y_1	5	Y_2
	3	Z_1	6	Z_2

2. Tetrahedron



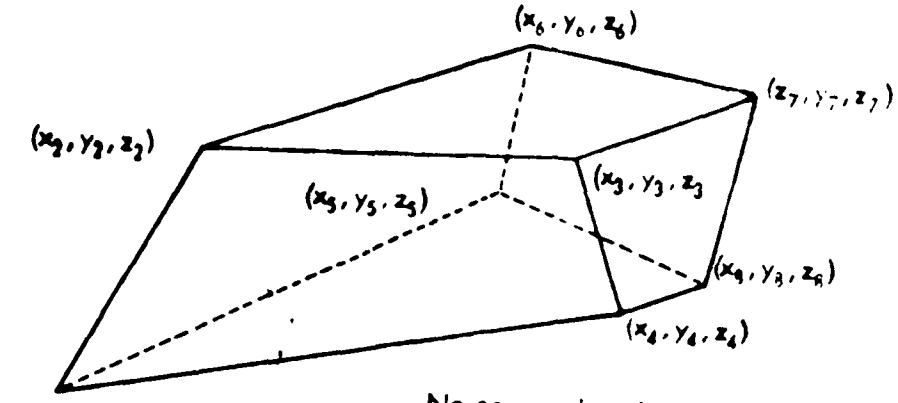
Code No.	79/89 Card Variables			
72 - insert	1	X_1	6	Z_2
82 - delete	2	Y_1	7	X_3
	3	Z_1	8	Y_3
	4	X_2	9	Z_3
	5	Y_2		

3. Ellipsoid



Code No.	79/89 Card Variables			
73 - insert	1	X_0	4	a
83 - delete	2	Y_0	5	b
	3	Z_0	6	c

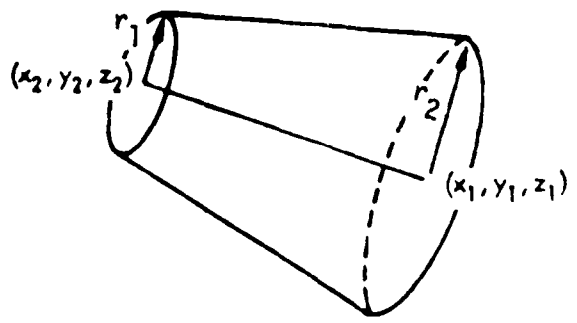
4. Irregular solid figure bounded by quadrilaterals



No convex interior angles

Code No.	79/89 Card Variables			
74 - insert	1	X_1	13	X_5
84 - delete	2	Y_1	14	Y_5
	3	Z_1	15	Z_5
	4	X_2	16	X_6
	5	Y_2	17	Y_6
	6	Z_2	18	Z_6
	7	X_3	19	X_7
	8	Y_3	20	Y_7
	9	Z_3	21	Z_7
	10	X_4	22	X_8
	11	Y_4	23	Y_8
	12	Z_4	24	Z_8

5. Frustum of cone



Code No.	79/89 Card Variables			
75 - insert	1	X_1	5	Y_2
85 - delete	2	Y_1	6	Z_2
	3	Z_1	7	r_1
	4	X_2	8	r_2

Note: This will require two 79/89 cards.

Material Properties Fits

In most cases, the material properties within a given geometrical shape will be uniform in the initial zoning. Special cases might be encountered which require variation within the shape. Provisions are available to treat this situation though special coding will normally be required.

If this special fit is used (NFIT = 1 on Card 10.1) insert cards below instead of Cards 10.7 to 10.10. Normally used with shape option No. III.

Fit No. 1

$$\text{Let } \xi = \sqrt{(X - X_0)^2 + (Y - Y_0)^2 + (Z - Z_0)^2}$$

$$\rho = C_1 + C_2\xi^2$$

$$T = C_3 + C_4\xi$$

$$V_y = C_5 (Y - Y_o)$$

$$V_x = C_6 (X - X_o)$$

$$V_z = C_7 (Z - Z_o)$$

Card	Variable Following Card Identification Number	Constant
91	1	C_1
	2	C_2
	3	X_o
	4	Y_o
92	1	C_3
	2	C_4
93	1, 2, 3	C_5, C_6, C_7

No stress deviators are defined (94 card), i.e.,

$$\sigma^d_{zz} = \sigma^d_{yz} = \sigma^d_{xz} = \sigma^d_{xx} = \sigma^d_{xy} = \sigma^d_{yy} = 0, \text{ with Fit No. 1}$$

Card Set 10 — Insertion of material into mesh

Card 10.1	Format (5I5, A55)	Insert Material Option
Variable 1. (1-5)	Shape Code (71 to 74)	
Variable 2. (6-10)	NSUB	= Number of subdivisions in cell coordinates for zoning. (1 to 100 depending on resolution required). There are $NSUB^3$ subcells per cell. The center of each subcell is tested against the zoning package.

Variable 3. (11-15)	NDEL	= Number of delete package (80 maximum) to follow and applied against this insert package.
Variable 4. (16-20)	KEOS	= Material type indicator 0 = void — 0 would be used to define a hot spatial region, i.e., hot void >0 for material KEOS. (Material KEOS uses EOS number NEOS(KEOS) as on card 2.)
Variable 5. (21-25)	NFIT	= 0 for uniform region material properties. $\geq$ 1 = Fit number for nonuniform material properties (see previous material properties fits disdussion). Two fits are presently coded as examples (NFIT = 1 and 707)
Variable 6. (26-80)	Any BCD information for comment.	

Card 10.2	Format (I5, 5X, 6E10.3)	Shape Dimensions
Variable 1. (1-5)	Integer 79	
Variable 2 to 7. (11-70)	Shape variables 1 to 6 (See previous Shape Options Section)	

Card 10.3	Format (I5, 5X, 2E10.3)	Continuation of last card

Used only with shape option IV.

Variable 1. (1-5)	Integer 79
Variables 2 and 3. (11-30)	Shape variable 7 and 8

Note: Cards 10.4 - 10.6 are present only if NDEL > 0 on Card 10.1. If NDEL > 0, there are NDEL sets of Card 10.4 to 10.6.

Card 10.4	Format (I5)	Delete for last insert package
Variable 1. (1-5)	Shape Code (81 to 84)	

Cards 10.5 and 10.6

Same as Card 10.2 and 10.3 except code is 89 instead of 79.

Note: See Material Properties Fits for Cards 10.7 to 10.10 if NFIT on Card 10.1 is greater than zero. Any of the cards with identification number 91 to 94 can be left out if a zero or default input is desired. They can be in any order. Card 10.11 (identification number 90) must always be present.

Card 10.7	Format (I5, 5X, 7E10.3)	Density
Variable 1. (1-5)	Integer 91	
Variable 2. (11-20)	ρ = material density	

Card 10.8	Format (I5, 5X, 7E10.3)	Temperature or Pressure
Variable 1. (1-5)	Integer 92	
Variable 2.	T = material temperature [if $T \leq 0$ code sets T = 0.02567785 ev (298°K)]	

OR

Variable 1. (1-5)	Integer 92	
Variable 2. (11-20)	P = material pressure (dynes/cm^2)	
Variable 3. (21-30)	1. (flag)	

Card 10.9	Format (I5, 5X, 7E10.3)	X, Y and Z Velocities
Variable 1. (1-5)	Integer 93	
Variable 2. (11-20)	V_x = X velocity of material	
Variable 3. (21-30)	V_y = Y velocity of material	
Variable 4. (31-40)	V_z = Z velocity of material	

Card 10.10*	Format (I5, 5X, 7E10.3)	Stress Deviators
Variable 1. (1-5)	Integer 94	
Variable 2. (11-20)	σ^d_{xx}	
Variable 3. (21-30)	σ^d_{yy}	
Variable 4. (31-40)	σ^d_{zz}	
Variable 5. (41-50)	σ^d_{xy}	
Variable 6. (51-60)	σ^d_{yz}	
Variable 7. (61-70)	σ^d_{xz}	

*Card 10.10 should only be used if NELEP = 1 on Card 4.

Card 10.11	Format (I5)	Stop card (must be present)
Variable 1. (1-5)	Integer 90	

If NFIT = 707 (Card 10.1), insert Card Set G here. See discussion at end of K3GEN instructions.

To define more material regions go to Card 10.1 and start over. When finished insert Card 10.12.

Card 10.12	Format (I5)	Stop card
Variable 1. (1-5)	Integer 70	

Card Set G Stable configuration with gravity

This set of cards is used to define a stable configuration in a gravitational field (Y direction only). The information is used by the material properties calculation for NFIT = 707 (Card 10.1 in K3GEN). When present, this card set follows the 90 card (Card 10.11 in K3GEN). There can be several sets of these cards; one for each material insert package desired. If there are several sets of these cards, care must be used to insure proper top and bottom pressures.

Card G.1	Format (I5, 5X, 6E10.3)
Variable 1. (1-5)	Integer 707
Variable 2. (11-20)	YB = smallest Y for package
Variable 3. (21-30)	PB = pressure at YB†
Variable 4. (31-40)	YT = largest Y for package
Variable 5. (41-50)	PT = pressure at YT†
Variable 6. (51-60)	T For a constant temperature atmosphere, insert temperature. If T = 0, code set T = .02567785. For an altitude dependent temperature, insert a negative number and Card Set G.2.
Variable 7. (61-70)	RHOG = approximate density at boundary with defined pressure for starting iterations.

† Define either PB or PT and leave other blank.

Card Set G.2 Format (I5, 5X, 2E10.3) Temperature - Altitude Relation

Present only if T < 0 (Variable 6 on Card G.1).

Insert one card for each desired point. Start at bottom of mesh and work upward. Stop with Card G.3.

Variable 1. (1-5)	Integer 701	
Variable 2. (11-20)	Y	For following temperature.
Variable 3. (21-30)	Temperature	

Card G.3 Format (I5) Stop Card

Present only if Card Set G.2 is used.

Variable 1. (1-5)	Integer 700

b. ANEOS Input Cards

The equation-of-state input data information presented here is reproduced from Reference 1 for the convenience of the user. This information can also be found in Appendix F of Reference 4.

The card set forms the necessary data cards for Card Set 3 in K3GEN, Card Set 12 in CHART D, Card Set 2 in CKEOS2 and any other program which uses the ANEOS equation-of-state package. Note that there are 8 optional forms with 4 different input formats. The first variable on the first card of each form must agree with the data on Card 2 of K3GEN.

Inputs for ANEOS options 0 to +4

Card 1.	Format (I3, I5, I2, 5A10, 2E10.3)
Variable 1. (1-3)	Equation-of-state number (negative number). -1 to -10 for K3GEN
Variable 2. (4-8)	Library equation-of-state number if desired; otherwise zero.†
Variable 3. (9-10)	Used only with a library equation-of-state. This variable determines the type of analytic calculation (see variable 2, card 2 below). If out of range 0 to 4, or library information is only for a gas, this input is ignored.
Variable 4 - 8. (11-60)	Fifty-column identification label: any BCD information.
Variable 9. (61-70)	RHUG - The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density (variable 3, card 2 below).

† See Appendix C in R3 for contents.

Variable 10. (71-80) THUG - The initial temperature for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below).

If a library equation of state is requested, no further data cards are required.

Cards 2, 3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. (1-10) The number of elements in this material.

Variable 2. (11-20) Switch for type of equation-of-state. See Reference 8 for these options.

0. - Solid-gas without electronic terms and without detailed treatment of the liquid-vapor region.
1. - Solid-gas with electronic terms but without detailed treatment of the liquid-vapor region.
2. - Gas only with electronic terms.
3. - Same as 0., but with a detailed treatment of the liquid-vapor region.
4. - Same as 1., but with a detailed treatment of the liquid-vapor region.

Variable 3. (21-30) ρ_0 - Reference density.

Variable 4. (31-40) T_0 - Reference temperature
If $T \leq 0$, code sets T_0 = 0.02567785 ev (298°K).

Variable 5. (41-50) P_0 - Reference pressure (normally 0).

Variable 6. B_0 - Reference bulk modulus (positive number)
or
$(-S_0)$ - Constant in linear Hugoniot shock-particle velocity relation (negative number)

Variable 7. (61-70)

Γ_o - Reference Grüneisen coefficient.

Variable 8. (71-80)

$\pm\theta_o$ - Reference Debye temperature.

If $\theta_o = 0$, code sets $\theta_o = 0.025$.

If $\theta_o > 0$, use high temperature approximation

If $\theta_o < 0$, calculate complete Debye functions

Variable 9. (1-10)

T_Γ - Parameter for selection of model.

$T_\Gamma = -1$, Slater theory,

$T_\Gamma = 0$, Dugdale and MacDonald theory,

$T_\Gamma = 1$, free-volume theory,

or

S_1 - Constant in linear Hugoniot shock-particle velocity relation. Input variable is defined in relation to variable 6.

Variable 10. (11-20)

$3C_{24}$ - Three times the limiting value of the Grüneisen coefficient for large compressions, usually either 2 or 0.

When a value of 2 is used, $C_{24} = 2/3$.

Variable 11. (21-30)

E_s - Zero temperature separation energy.

Variable 12. (31-40)

T_m - Melting temperature (positive number)

or

$(-E_m)$ - Energy to the melting point at zero pressure from the reference point (negative number).

Variable 13. (41-50)

C_{53} - Parameter for low density P_c modification to move critical point (normally zero).

Variable 14. (51-60) — C_{54} - Parameter for low density P_c modification to move critical point (normally zero).

If $C_{54} = 0$ and $C_{53} \neq 0$, codes sets $C_{54} = 0.95$.

Variable 15. (61-70) — H_o - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $H = H_o T^{C41}$ are ergs/(cm sec eV).

Variable 16. (71-80) — C_{41} - Temperature dependence of thermal conduction ccoefficient (see variable 15).

Variable 17. (1-10) — ρ_{min} - Lowest allowed solid density, usually about $0.8\rho_o$. If zero or negative, code sets $\rho_{min} = 0.8\ \rho_o$.

Variable 18. (11-20) — Parameter D_1

Variable 19. (21-30) — Parameter D_2

Variable 20. (31-40) — Parameter D_3

Variable 21. (41-50) — Parameter D_4

Variable 22. (51-60) — Parameter D_5

} Solid-solid phase transition parameters (normally 0).

Variable 23. (61-70) — H_f - Heat of fusion to determine melt transition parameters.
If $H_f = 0$, no transition is included.
If $H_f < 0$, code sets $H_f = 1.117 \times 10^{12}\ T_m/A$(ergs/gm), where A is the average atomic weight.

Note: Code will run slower if the melt transition is included. Use only when necessary and after testing.

Variable 24. ρ_ℓ/ρ_s - Ratio of liquid to solid density at melt point
or
$(-\rho_\ell)$ - Density of liquid at melt point.
or
$1 + \Delta V = 1 + V_\ell - V_s$ - Change in volume at melt plus one.
Note: In the first option, the input number is between 0 and 1; in the second it is negative; and in the third greater than one.
If $H_f \neq 0$ and $\rho_\ell/\rho_s = 0$, code sets $\rho_\ell/\rho_s = 0.95$.

For a gaseous equation of state (type 2), variables 5 to 14 and 17 to 24 are read but not used.

Card 5 Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable 1, card 2.

I = 1, number of elements.

Variable Odd. Z(I) - Atomic number of element.

Variable Even. Unnormalized atomic number fraction of element [COT(I)].
or
- (Unnormalized atomic weight fraction of element.)
All elements should be defined in the same way.

Inputs for ANEOS Option -1

Card 1. Format (I3, I5, I2, 5A10, 2E10.3)

Variable 1. (1-3) Equation-of-state number (negative number).

Variable 2. (4-8) Library equation-of-state number if desired; otherwise zero.

Variable 3. (9-10)	Used only with a library equation-of-state. This variable determines the type of analytic calculation (see variable 2, card 2 below). Must be -1 in this case.
Variable 4 - 8 (11-60)	Fifty-column identification label: any BCD information.
Variable 9 (61-70)	RHUG = The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density (variable 3, card 2 below).
Variable 10.	THUG = The initial temperature for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below).
	If a library equation-of-state is requested, no further data cards are required.

Cards 2, 3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. (1-10)	The number of elements in this material.
Variable 2. (11-20)	Switch for type of equation of state. Must be -1 for this option.
Variable 3. (21-30)	ρ_0 - Reference density.
Variable 4. (31-40)	T_0 - Reference temperature. If $T_0 \leq 0$, code sets T_0 = 0.02567785 eV (298°K).
Variable 5. (41-50)	Blank.

Variable 6. (51-60)	S_0 - Reference point bulk sound speed.
Variable 7. (61-70)	Γ_0 - Reference Gruneissen coefficient.
Variable 8. (71-80)	Blank.
Variable 9. (1-10)	S_1 - Constant in linear Hugoniot shock-particle velocity relation. or (-100) - For power series representation of P_H Enter variables 18 to 21 or ($-S_1$ -100) - For power series representation with S_1 for low density.
Variable 10. (11-20)	Blank.
Variable 11. (21-30)	C_v - Heat capacity. If $C_v \leq 0$, code sets C_v = 3 No. k.
Variable 12. (31-40)	T_m - Melting temperature (positive number) or ($-E_m$) - Energy to the melting point at zero pressure from the reference point (negative number).
Variable 13. (41-50)	Blank.
Variable 14. (51-60)	Blank.
Variable 15. (61-70)	H_0 - Thermal conductivity coefficient. If zero, thermal conduction is not included. Note that the units of $H = H_0 T^{C41}$ are ergs/(cm sec eV).

Variable 16. (71-80)	C_{41} - Temperature dependence of thermal conduction coefficient (see variable 15).
Variable 17. (1-10)	ρ_{min} - Lowest allowed solid density, usually about $0.8\rho_o$. If zero or negative, code sets $\rho_{min} = 0.8\rho_o$.
Variable 18. (11-20)	K_1.
Variable 19. (21-30)	K_2. Constants in power series representation of P_H.
Variable 20. (31-40)	K_3. Enter only if variable 9 $\leq$ -100. Blank otherwise.
Variable 21. (41-50)	K_4.
Variable 22. (51-60)	Blank.
Variable 23. (61-70)	Blank.
Variable 24. (71-80)	Blank.

Card 5 Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable 1, card 2.

1 = 1, number of elements.

Variable Odd.	Z(I) - Atomic number of element.
Variable Even.	Unnormalized atomic number fraction of element [COT(I)]. or -(Unnormalized atomic weight fraction of element.) All elements should be defined in the same way.

Inputs for ANEOS Option -2

Card 1. Format (I3, I5, I2, 5A10, 2E10.3)

Variable 1. (1-3)	Equation-of-state number (negative number).
Variable 2. (4-8)	Library equation-of-state number if desired; otherwise zero.
Variable 3. (9-10)	Used only with a library equation-of-state. This variable determines the type of analytic calculation (see variable 2, card 2 below). Must be -2 in this case.
Variable 4 - 8. (11-60)	Fifty-column identification label: any BCD information.
Variable 9. (61-70)	RHUG = The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density (variable 3, card 2 below).
Variable 10. (71-80)	THUG = The initial temperature for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below).
	If a library equation-of-state is requested, no further data cards are required.

Cards 2, 3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. (1-10)	The number of elements in this material.
Variable 2. (11-20)	Switch for type of equation-of-state. Must be -2 for this option.
Variable 3. (21-30)	ρ_0 - Reference density.

Variable 4. (31-40)	T_o - Reference temperature. If $T_o \leq 0$, code sets T_o = 0.02567785 eV (298°K).
Variable 5. (41-50)	K_1 - Constant in Rosseland opacity expression. Units are cm^2/gm.
Variable 6. (51-60)	Blank.
Variable 7. (61-70)	$(\gamma - 1)$ - Specific heat ratio minus one.
Variable 8. (71-80)	K_2 - Constant in Rosseland opacity expression Units are eV. If $K_2 \leq 0$, code sets K_2 = .025 eV.
Variable 9. (1-10)	Blank.
Variable 10. (11-20)	Blank.
Variable 11. (21-30)	C_v - Heat capacity. If $C_v \leq 0$, code sets C_v = 3/2 No k.
Variable 12. (31-40)	Blank.
Variable 13. (41-50)	Blank
Variable 14. (51-60)	Blank.
Variable 15. (61-70)	Blank.
Variable 16. (71-80)	Blank.
Variable 17. (1-10)	Blank.

Variable 18. (11-20)	Blank.
Variable 19. (21-30)	Blank.
Variable 20. (31-40)	Blank.
Variable 21. (41-50)	Blank.
Variable 22. (51-60)	Blank.
Variable 23. (61-70)	Blank.
Variable 24. (71-80)	Blank.

Card 5. Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable 1, card 2.

I = 1, number of elements.

Variable Odd.	Z(I) - Atomic number of element.
Variable Even.	Unnormalized atomic number fraction of element [COT(I)], or -(Unnormalized atomic weight fraction of element.) All elements should be defined in the same way.

Inputs for ANEOS Option -3

Card 1. Format (I3, I5, I2, 5A10, 2E10.3)

Variable 1. (1-3)	Equation-of-state number (negative number).

Variable 2. (4-8)	Library equation-of-state number if desired; otherwise zero.
Variable 3. (9-10)	Used only with a library equation-of-state. This variable determines the type of analytic calculation (see variable 2, card 2 below). Must be -3 in this case.
Variables 4 - 8 (11-60)	Fifty-column identification label: any BCD information.
Variable 9. (61-70)	RHUG - The initial density for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial density is taken to be the reference density, (variable 3, card 2 below).
Variable 10. (71-80)	THUG = The initial temperature for the Hugoniot calculation. If zero, the calculation is skipped. If negative, the initial temperature is taken to be the reference temperature (variable 4, card 2 below).
	If a library equation-of-state is requested, no further data cards are required.

Cards 2, 3, and 4 Format (8E10.3)

In the listing, the following variables are called ZB(I), I = 1, 24.

Variable 1. (1-10)	The number of elements in this material.
Variable 2. (11-20)	Switch for type of equation-of-state. Must be -3 for this option.
Variable 3. (21-30)	ρ_0 - Reference density.
Variable 4. (31-40)	T_0 - Reference temperature. If $T \leq 0$, code sets T_0 = 0.02567785 eV (298°K).

Variable 5. (41-50)	K_1 - Constant in Rosseland opacity expression. Units are cm^2/gm.
Variable 6. (51-60)	1. - Integer which must be entered but not used.
Variable 7. (61-70)	ω - LLL constant. (See variable 18 below).
Variable 8. (71-80)	K_2 - Constant in Rosseland opacity expression. Units are eV. If $K_2 \leq 0$, code sets K_2 = 0.25 eV.
Variable 9. (1-10)	Blank.
Variable 10. (11-20)	Blank.
Variable 11. (21-30)	C_v - Heat capacity. If $C_v \leq 0$, code sets C_v = 3 No k.
Variable 12. (31-40)	T_m - Melting temperature (positive number) or $(-E_m)$ - Energy to the melting point at zero pressure from the reference point (negative number).
Variable 13. (41-50)	Blank.
Variable 14. (51-60)	Blank.
Variable 15. (61-70)	H_o - Thermal conductivity coefficient. If zero, conduction is not included. Note that the units of $H = H_o T^C 41$ are ergs/(cm sec eV).

Variable 16. (71-80)	C_{41} - Temperature dependence of thermal conduction coefficient (see variable 15).
Variable 17. (1-10)	ρ_{min} - Lowest allowed solid density, usually about 0.8 ρ_o. If zero or negative, code sets ρ_{min} = 0.8 ρ_o.
Variable 18. (11-20)	A.
Variable 19. (21-30)	B.
Variable 20. (31-40)	R_1
Variable 21. (41-50)	R_2

LLL Constants. (see reference 6)

Variable 22. (51-60)	Blank.
Variable 23. (61-70)	Blank.
Variable 24. (71-80)	Blank.

Card 5. Format (5(F5.0, E10.3))

There is one set of the following variables for each element in variable 1, card 2.

I = 1, number of elements. See reference 7 for element table.

Variable Odd.	Z(I) - Atomic number of element.
Variable Even.	Unnormalized atomic number fraction of element [COT(I)]. or -(Unnormalized atomic weight fraction of element.) All elements should be defined in the same way.

3. K3

K3 is the main computation program. It requires a variable amount of central memory storage (CM) and extended core storage. The CM varies even for fixed mesh size since there are five sets of optional subroutine packages which need to be loaded only when specialized calculations are used. These are:

1. elastic-plastic package
2. energy-flow package
3. energy source/high explosive package (not operational)
4. mesh fix package (not operational)
5. material history package (not operational)

It should be obvious which packages are required for a given computation.

The following suggestions are included to aid the user. Their meaning will be clearer after going through the input instructions.

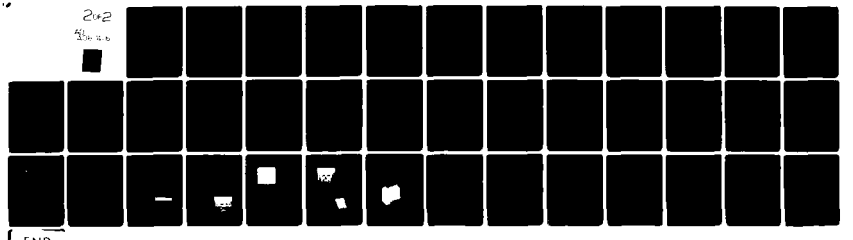
1. Each run by K3 is considered as a restart of a previous run. K3GEN must be employed to generate the first restart dump for input unit 1 (dump number 1).
2. Cell centers are tested to determine if a cell is inside a region defined as an energy source.
3. If the program immediately has an address out of range error (MODE = 1), check optional subroutine packages above.

Tape Units K3

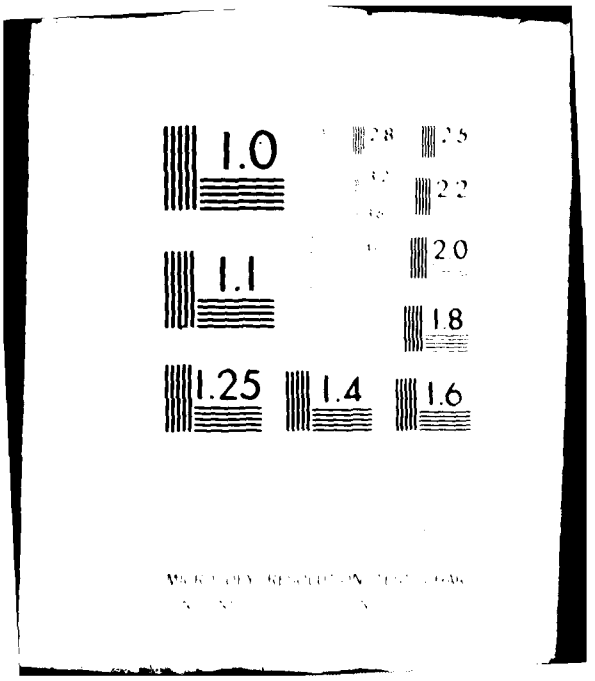
1. Restart input tape and standard restart output tape (must be present).
2. Optional restart output tape.
3. Plot output tape.
55. Material history output tape.
67. Internal storage.
77. Internal storage.

Note: Both restart and plot tapes have identical formats. The program can be restarted from a plot tape or plots can be made from a restart tape.

AD-A087 416 KAMAN SCIENCES CORP COLORADO SPRINGS COLO F/G 19/4
K3. AN EULERIAN FINITE DIFFERENCE PROGRAM FOR THREE-DIMENSIONAL--ETC(U)
FEB 80 J MAY, P SNOW, D C WILLIAMS DAS660-79-C-0098
UNCLASSIFIED K-80-226(R) NL



END
DATE FILMED
9-80
DTIC


1.0
1.1
1.25
1.4
1.6
2.2
2.0
1.8

K3 Inputs

Card 1.	Format (7A10, I10)	
(1-70)	BCD title (MUST agree with 1-40 in title defined in K3GEN, 41-70 can be changed).	
(71-80)	NSTART	- Restart tape dump number to begin run. (No. from K3GEN is one) Following restart dumps are added to the tape after the last one read to start run. This can be changed by variable 10 on card 2. If NSTART < 0 code will read to the last dump on the tape and start from there. If NSTART = 0 code sets NSTART = 1.

Card 2.	Format (E10.3, 1415)	
Variable 1. (1-10)	TSTOP	= problem stop time* If TSTOP = 0, code sets TSTOP = ∞.
Variable 2. (11-15)	ICYCLES	= problem stop cycle* If ICYCLES = 0, code sets ICYCLES = ∞.
Variable 3. (16-20)	MEDITS	= ± number of short print intervals in card set 4. $0 < \|MEDITS\| \leq 9$
Variable 4. (21-25)	MEDIT	= ± number of long print intervals in card set 5. $0 < \|MEDIT\| \leq 9$
Variable 5. (26-30)	MOVIE	= ± number of plot dump intervals in card set 6. $0 \leq \|MOVIE\| \leq 9$
Variable 6. (31-35)	NDUMPF	= seconds of C.P. time between restart tape dumps. If NDUMPF $\leq$ 0 code sets NDUMPF = 3600 sec.
Variable 7. (36-40)	NDTMAX	= number of Δt_{max} intervals in card set 7. $0 \leq NDTMAX \leq 9$

* Program will terminate on the computer C.P. clock if TSTOP and ICYCLES are not defined.

Variable 8. (41-45) NDTMIN = number of Δt_{min} intervals in card set 8. $0 \leq$ NDTMIN ≤ 9

Variable 9. (46-50) NTBOUND = number of radiation boundary temperatures to be defined (not operational).

Variable 10. (51-55) NREST = restart output switch
If NREST = 0, output tape is 1 (same as restart input)
If NREST $\neq$ 0, output tape is 2.

Variable 11. (56-60) KNARRX = switch for card set 9.
If $\leq$ 0, no card set 9
If > 0, allows change of any variable in integer common block with card set 9.

Variable 12. (61-65) KARRX = switch for card set 10.
same as KNARRX except for floating common block and card set 10.

Variable 13. (66-70) NEXTV1 = print switch for nonstandard edit variable.. See card 4 in K3GEN inputs but here one inputs the value of the zone storage order variable, i.e., value of LK(NEXTV1) as in K3GEN. Use only if it is desired to change K3GEN inputs.

Variable 14. (71-75) NEXTV2 = same as NEXTV1 for second printed variable.

Variable 15. (76-80) NEXTV3 = same as NEXTV1 for third printed variable.

Card 3. Format (4F5.0, E10.3, 9F5.0)

Variable 1. (1-5) SOURCES = switch for energy sources
= 0 no sources
= 1 input source data (not operational)

Variable 2. (5-10)	ELPL	= switch for elastic-plastic calculation. = 0 to turn off EP calculation. $\geq$ 1 EP calculation on and card set 12 is required. The value of ELPL determines how yield functions are treated in a mixed cell. = 1, volume average yield parameters (normal) = 2, $\sigma^d_{xz} = 0$ in mixed cell. = 3, Y = 0 in mixed cell.
Variable 3. (11-15)	POROUS	Not Used
Variable 4. (16-20)	FRACT	= switch for input of fracture calculation data. See card set 11. If FRACT $\neq$ 0 input card set 11. If FRACT = 1 input pressures. If FRACT = 2 input stresses.
Variable 5. (21-30)	GRAV	= acceleration of gravity (980 cm/sec) if desired; zero otherwise. (acceleration in - Y direction only).
Variable 6. (31-35)	PRINTO	= switch to control long edit on 1st cycle of current run = 0 long edit on 1st cycle $\neq$ 0 no long print of 1st cycle (but gives short edit).
Variable 7. (36-40)	CPSHIFT	= variable to allow for extra CP time in seconds in computer clock run termination. Used to allow time for tape copying, plots, etc. Default value is 15.
Variable 8. (41-45)	FNTRACE	= switch to allow changes in tracer particle position = 0. no change $\neq$ 0. input data (not operational).

Variable 9. (46-50)	EXTAPM	= switch to allow continuation of plot output file on previously generated reel (unit 3). See variable 5, card 2 and card 6. = 0, generate new file on output unit 3 > 0, add new data after data generated during a previous run. EXTAPM is the last cycle number to be retained from old data. Cycles with cycle number > EXTAPM are overwritten. < 0. add new data after last cycle dump on the old file. (EXTAPM = 0 for cycle 0 always)
Variable 10. (51-55)	FRACDT	- Fraction of Courant stability used to calculate Δt_{cs}. Normally 0.6, in no case greater than one. If FRACDT $\leq$ 0, code sets FRACDT = 0.6.
Variable 11. (56-60)	DTINCR	- Maximum factor allowed for increase in Δt from one cycle to the next. If DTINCR $\leq$ 0, code sets DTINCR = 1.068000433
Variable 12. (61-65)	FIXMH	- Switch to allow definition of fixed mesh lines. = 0, not used. $\neq$ 0, input data (not operational)
Variable 13. (66-70)	HIST	= Switch for output on history data tape (unit 55). = 0, no output $\neq$ 0, output data to tape 55. Output frequency is every $\lvert HIST \rvert^{\underline{th}}$ cycle. (Not operational)
Variable 14. (71-75)	RHOED	- Switch for extended long edit giving density and volume fraction for each material. = 0. no extended edit = 1. produce extended edit (used only if more than two materials present.)

Card Set 4 — Short Print Interval

Use either 4.1 or 4.2 depending on MEDITS on card 2. There are |MEDITS| sets of data pairs.

If MEDITS > 0

Card 4.1 Format (8E10.3)

I = 1, MEDITS

Variable Odd -	PTIMES(I)	= time at which the short edit frequency changes from DPTIMES(I-1) to DPTIMES(I). [PTIMES(1) $\leq$ start time of problem]
Variable Even -	DPTIMES(I)	= the time interval between short edits from PTIMES(I) to PTIMES(I+1)

For times > PTIMES(MEDITS), interval DPTIMES(MEDITS) is used to the end of the calculation.

If MEDITS < 0

Card 4.2 Format (8I10)

Same as 4.1 except cycles are used instead of time. The variables are named NCYEDS(I) and NDCYEDS(I).

Card Set 5 — Long Print Interval

Use either 5.1 or 5.2 depending on MEDIT on card 2. There are |MEDIT| sets of data pairs. A short edit is always given as part of the long edit.
Warning---long edits are long for large problems.

If MEDIT > 0

Card 5.1 Format (8E10.3)

Same as card 4.1 except for long edit. The variable names are PTIME(I) and DPTIME(I).

If MEDIT < 0

Card 5.2 Format (8I10)

Same as card 4.2 except for long edit. The variable names are NCYED(I) and NDCYED(I).

Card Set 6 Plot Tape Dump Intervals

Present only if MOVIE ≠ 0 on card 2.

Use either 6.1 or 6.2 depending on MOVIE on card 2. There are |MOVIE| sets of data pairs.

If MOVIE > 0

Card 6.1 Format (8E10.3)

Same as card 4.1 except for plot tape dumps. The variable names are TMOVIE(I) and DTMOVIE(I).

If MOVIE < 0

Card 6.2 Format (8I10)

Same as card 4.2 except for plot tape dumps. The variable names are IMOVIE(I) and IDMOVIE(I).

Card Set 7 Format (8E10.3) Δt_{max} data

Present only if NDTMAX > 0 on card 2.

Same form as card 4.1. The variable names are TDTMAXX(I) and DTMAXX(I).

Card Set 8 Format (8E10.3) Δt_{min} data

Present only if NDTMIN > 0 on card 2.

Same form as card 4.2. The variable names are TDTMINN(I) and DTMINN(I).

Card Set 9 Format (2I10)

Present only if KNARRX > 0 on card 2.

This card set allows the changing of a variable(s) in the integer COMMON block.* CAREFUL

Variable 1. (1-10)	I	= location in NARRX array.
Variable 2. (11-20)	NARRX(I)	= new value to put in location NARRX(I)

Repeat cards until finished.

Insert blank card to stop reading these cards.

Card Set 10. Format (I10, E10.3)

Present only if KARRX > 0 on card 2.

This card set allows the changing of a variable(s) in the floating COMMON block.* CAREFUL

Variable 1. (1-10)	I	= location in ARRX array.
Variable 2. (11-20)	ARRX(I)	= new value of ARRX(I).

Repeat cards until finished. Insert blank card to stop reading these cards.

---

*For example IACT = NARRX(17)

TIME = ARRX(33)

Card Set 11. Fracture Data

Present only if FRACT ≠ 0 on card 3.
If FRACT = 1, all inputs are pressure values.
If FRACT = 2, all inputs are stress values except for $P_{fRACT\ VOID}$ which is pressure. All quantities are negative and in units of dynes/cm^2. Default values [] are used for any zero input value or if FRACT = 0. Since positive numbers have no meaning in the present model, the code will add the minus if a positive number is found.

Card 11.1	Format (8E10.3)	
Variables K = 1,..., NUMMT	$P_{FRACT}(K)$	= minimum stress or pressure in a cell of material K with no void present. There is one input for each material. [$-2x10^{10}$]
Variable	$P_{FRACT\ MIX}$	= minimum stress or pressure in a cell of mixed material with no void present. Inputs on card 11.2 will override this variable for special mixtures. [$-1x10^{8}$]
Variable	$P_{FRACT\ VOID}$	= minimum pressure in any cell containing void. [$-5x10^{6}$]
Variable	NFACES	= number of cards 11.2 to define interface strengths. An integer but punched with decimal point 0. ≤ NFACES ≤ 12. (floating number)

Continue on card with identical format for 6 or more materials.

Card 11.2	Format (2I5, E10.3)	

There are NFACES (card 11.1) of these cards to define strength at material interfaces between any two materials. I = 1, NFACES

Variable 1. (1-5)	MATF1	= one of materials at interface
Variable 2. (6-10)	MATF2	= other material at interface
Variable 3. (11-20)	P_{FRACT}	= minimum stress or pressure in a cell containing only materials MATF1 and MATF2. (no void or other materials) [$P_{fRACT\ MIX}$]

Card Set 12. Format (7E10.3) Elastic Properties

Present only if ELPL > 0 on card 3.

The elastic-plastic package of subroutines must be loaded with K3 if this option is used.

SHOULD be included for EP calculation

There is one of the following cards for each of the NUMMT materials. Material 1 first, etc. Input blank card for hydrodynamic material.

Variable 1. (1-10) Y_0 (dynes/cm^2)

Variable 2. (11-20) ε_m = absolute value of melt energy (ergs/gm)
If not defined, the program will determine for EOS.

Variable 3. (21-30) ν_0 = Poisson ratio.

Variable 4. (31-40) C_{smin} = minimum bulk sound velocity to be used to calculate shear modulus. (normally zero)

Variable 5. (41-50) α = fraction of melt energy where material begins to lose strength.
If $\alpha \leq 0$, code sets $\alpha = 0.8$

Variable 6. (51-60) RHOEPU = ρ_u. If $\rho_j \leq 0$, code sets $\rho_u = 0.9\ \rho_m$, where ρ_m is the liquid density at zero pressure melt.

Variable 7. RHOEPL = ρ_L. If $\rho_L \leq 0$, coee sets $\rho_L = 0.9\ \rho_L$.

Card Set 13. Reserved for future expansion.

4. K3PLT

a. General

K3PLT is a program used to produce dot plots on the U.S. Army's Advanced Research Center's interactive color graphics system. (See Reference 5 for a description of the system and operating instructions). K3PLT is a modification of CSQPLT and the SCORS support plotting package and produces a two-dimensional image of selected parameters edited from K3 restart/dump tapes. The main use of K3PLT is to produce material density plots but can also, without modification, plot pressure or temperature. A subroutine OPUS is provided allowing the user to modify the program with minimal effort in order to select other parameters for plotting.

The amount of extended core storage (ECS) currently programmed into K3PLT for storage of plot variables in 100010. This amount can be increased or reduced, if desired, to suit problem requirements and thereby increasing program-computer efficiency. The amount of ECS required is 4*IMAX*JMAX*KMAX, but can get by with less, using disk file for excess storage requirements.

As stated above, K3PLT is an outgrowth of the CSQPLT program. The modifications made have negated some of the capabilities of the CSQPLT program and as a result, some inputs necessary for CSQPLT are no longer required for K3PLT. These inputs are included in the description of K3PLT for completeness sake, and in the event at some future time it is deemed useful to include the former capabilities.

b. Input Instructions

K3PLT is run interactively, with the user inputting control parameters via the system keyboard and trackball control. The following instructions lead the user step-by-step through the procedures necessary for obtaining pictures (plots) on the system's CRT.

Step 1 After job submittal a logo will appear on the screen of an available station, with a blinking cursor (the logo is currently "KAMAN SCIENCES CORPORATION" on a blue background). The cursor should be positioned onto the

lower quarter of the screen† using the trackball, and the trackball ENTER button depressed. This will advance the program to the next step, definition of inputs.

Step 2 The screen will display "ENTER DATA FOR CARD NO. 1" and "KON(**)=". The user should then enter the variable number (see Figure IV-1, list of card 1 inputs), via the keyboard, of KON that is to be changed from the default value. These inputs can be in any order desired. After the variable number is selected (which must be an integer), the screen will then display "KON(n*)=**********". The value of KON(n) should then be entered (which also must be an integer). The program will cease expecting values of KON when KON(16) is defined, or the user may skip to the next step by entering a slash (/) for any value of KON††. If the program is to be terminated, "ENDRUN" should be entered for any KON. Once the inputs are completed, the cursor will then blink, and the user may advance to the next step by depressing the trackball ENTER button†.

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† When the cursor is positioned in the upper three-quarters of the screen and the ENTER button depressed, the cursor position identifies the location at which alphanumeric data is to be entered from the keyboard (1 to 10 characters). This is handy for annotating plots for future identification. After entering the data (depressing the keyboard ENTER button), position the cursor to the lower portion of the screen and proceed.

†† For values of KON not defined, either the default values will be used, or values of KON previously defined.

KON	Default Value	Used	Description
1	1	Yes	= Input tape number (1-5)
2	0	No	= 0, display on CRT = 1, user tape 40 output
3	3	Yes	= 0, velocity vector (not available) = 1, momentum vector (not available) = 2, pressure = 3, density = 4, user option (see subroutine OPUS- temperature will be plotted as presently coded)
4	1	Yes	= 0, plot all tape dumps ≠ 0, plot only selected dumps (see also variables 13 and 14)
5	1	Yes	= number of mesh frames and number of dot scale frames ($\geq$ 0) - automatically reduced to zero after first plot
6	1	Yes	= number of title frames ($\geq$ 0)
7	1	Yes	= 0, no mirror image (in X direction) = 1, produce mirror image
8	1	Yes	= number of times to produce first plot ($\geq$ 1)
9	1	Yes	= number of times to produce following plots ($\geq$ 1)
10	0	No	= switch to plot interface lines/symbols (not available - should be zero)

Figure IV-1
K3PLT Inputs - Card Set 1

KON	Default Value	Used	Description
11	1	Yes	= number of THE END frames ($\geq$ 0)
12	0	No	= switch for frame size (not available - should be zero)
13*	1	Yes	= first tape dump to plot (see variable 4)
14*	20000	Yes	= last tape dump to plot (see variable 4)
15	0	No	= 0, produce dot plots $\geq$ 1, produce contour plots (not available)
16	0	No	= 0, do not plot tracer particles = 1, plot tracers with other plot data (not available) = -1, plot tracers without other plot data (not available)

* Program uses these inputs even if KON(4) is zero.

Figure IV-1 (continued)
K3PLT Inputs - Card Set 1

Step 3 The program will ask if the user wishes to define two titles for display on the title frame to be produced at a later stage of program execution. "YES" should be entered if the user wishes to enter titles on the first title frame. Any other entry will produce an unlabeled title frame (first title frame only) and advance the program to the next step. If titles are to be entered, the keyboard is used to enter the desired alphanumeric data. Again, once the program digests the user inputs, a blinking cursor signals that the program is waiting to be advanced.

Step 4 The screen will then display "ENTER DATA FOR CARD NO. 3" followed by XBL = **********". Refer to Figure IV-2 for the definition of these input variables. Entering a slash will automatically set the default values, or the values last used, for the displayed variable and any variables remaining to be defined for this input set. The values entered must be in floating print format, with or without an integer exponent. The following are examples of allowed inputs:

1.0
2.E-2
1.99999
-6.89E20

After all variables are defined, or a slash entered, the cursor will blink, and the trackball ENTER button should be depressed to advance to the next step.

Variable	Default	Description
XBL	0.0	X - left. (left-most value of abscissa) - automatically set to minus X - right if KON(7) is equal to 1.
XBR	0.0	X - right
YBB	0.0	Y - bottom
YBA	0.0	Y - top
ZBB	0.0	Z - back. Values of K-planes less than this will not be displayed
ZBF	0.0	Z - front. Values of K-planes greater than this will not be displayed
ROTA(1)*	0.0	Angle (in degrees) of X, Y, and Z rotation of density plots. X rotation is performed first followed by Y, then Z. Rotation is about the midpoint of X - left and X - right, Y - bottom and Y - top, Z - back and Z - front.
ROTA(2)*	0.0	
ROTA(3)*	0.0	
SCALEM	0.0	For velocity and momentum plots only - not available
VECTMIN	0.0	
DOTFM	2.0	Dot density control, given by $\left[\frac{\text{Variable}}{\text{DOTFM}}\right]^{\text{DOTPOW}}$ DOTPOW is restricted to $0. < \text{DOTPOW} \leq 1.0$
DOTPOW	1.0	

* if rotations are used, grid labeling is meaningless

Figure IV-2
K3PLT Inputs - Card Set 3

Step 5 If selected dumps are to be plotted (see definition of KON(4)), the program will expect the user to define the first dump to be plotted. Also, after the completion of each plot, the program will return to this step (if KON(4) is not zero) at which time the next dump to be plotted may be selected. If a zero is entered, the program will return to step 2, at which time the run may be terminated or new values of selected inputs may be entered. Note that dumps selected must be in ascending order - if a dump of lower numerical value is to be plotted, a return to step 2 must be made.

After the dump number is entered, the cursor will blink, and after the ENTER button is depressed, the program will initiate the actual plotting sequence.

c. Plots

The program will display a title frame, a mesh frame, and a plot of dot densities (if the appropriate KON values are non-zero) before the first dump is plotted. After each frame is displayed the cursor will blink signalling the frame is complete and the program is waiting before advancing to the next frame. This allows the user time to make hardcopy prints of the display or to study the screen. Advancement to the next frame is made by depressing the trackball ENTER button (see also the footnote with step 1).

The displays of selected dumps are built by displaying one K-plane at a time. The trackball cursor will blink after each plane is displayed. The ENTER button must be depressed to display the next K-plane. If the user wishes to terminate the display (not display any more K-planes for this plot) the trackball cursor can be positioned in the upper three-quarters of the screen, the ENTER button depressed, then the trackball cursor returned to the lower portion of the screen (where it will again blink, the program waiting to advance). After all K-planes have been displayed, or the display terminated by proper positioning of the trackball cursor, the program will return to step 5 if KON(4) is not zero or display the next dump. After all dumps have been displayed, a "THE END" frame will be displayed (if KON(11) is non-zero), and the program will return to step 2.

V. REFERENCES

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4. S.L. Thompson, Improvements in the CHART-D Energy Flow-Hydrodynamic Code V: 1972/1973 Modifications, SLA-73-0477, Sandia Laboratories, Albuquerque, New Mexico, October 1973.

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7. Properties of Chemical Explosives (By staff of Explosive Chemistry Section), UCRL-14592, Lawrence Livermore Laboratory, Livermore, California, December 1965.

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APPENDIX A

K3 TEST RUNS

K3 TEST RUNS

The purpose of this section is to provide the K3 user with

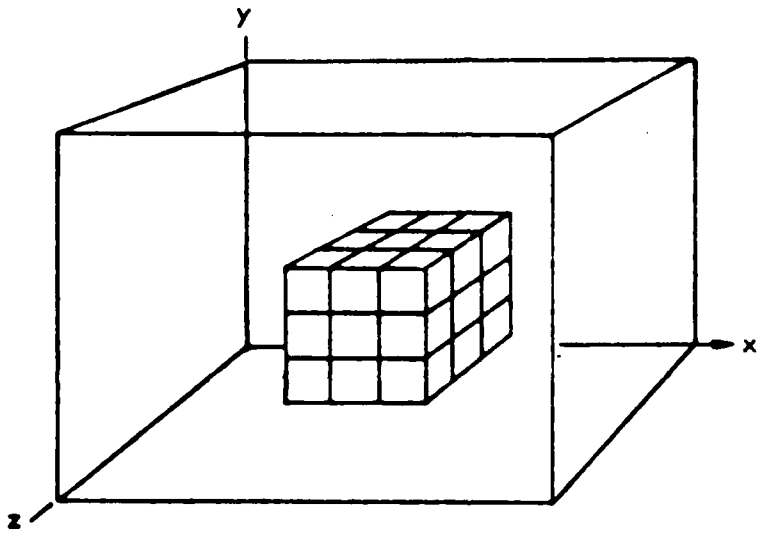
- o an overview of the runs made to test and debug the K3 family of programs,
- o example inputs for a specific problem,
- o example outputs from the K3PLT program

As can be imagined by those familiar with large program development, many unsuccessful test runs were made before satisfactory results were obtained. Plus, the test problems were set up, not necessarily to model a physically realistic situation, but rather to test out a specific portion of the code. These runs are not described here. What is described include, first, a series of runs made to test a) the symmetry of results, i.e., does the code predict material response and flow in a given direction consistent with that for the other directions, and b) that results are similar to those predicted by CSQ for the two-dimensional analog. These test runs were configured with a 27 cm^3 cube (three centimeters to a side) of high density gas situated in the center of a 7x7x7 centimeter box. The motion of the gas was observed as the gas expanded to fill the container.

Secondly, there is described a series of runs that were made with a physically realistic problem (indeed, the problem models an actual physical experiment) in order to compare results with those predicted with CSQ, to test out a large problem, and to test the completely assembled code. Since this last problem is of more interest than others, it is used to cover the last two items above, i.e., example inputs and outputs. The problem was to simulate the response of a block of aluminum with a steel backing plate impacted by a steel ball moving approximately 5000 meters per second.

1. Gas in a Box Problem

The initial configuration of the problem is shown in Figure A-1, where a 3x3x3 grid of gaseous material is placed in the center of a



3x3x3 Gas in 7x7x7 Grid
Reflective Boundary On all All Sides

Figure A-1. Gas-in-a-Box Configuration

7x7x7 grid box. Initially the sides of the box were solid to test boundary conditions. The reasons for choosing the above grid sizes were:

- o To reduce run time and amount of output by using the minimum size grid,
- o The minimum size of any active region should be at least 3 cells in any direction,
- o To provide space for the gas to expand, of a size to reduce computation time yet allow sufficient space to study movement from cell-to-cell before boundary contact,
- o Since CSQ in the Cartesian mode assumes a one centimeter thick cell in the imaginary z direction, one centimeter spacing for the entire grid was chosen to retain uniformity, for ease in interpreting output, and for direct comparison purposes.

The gas was polyethelene (this choice was arbitrary - any gas would have been sufficient for the problem) with a density of 2 grams/cm^3 and an internal pressure of 5×10^{12} dynes/cm^2. The total mass was 54 grams.

With the void fraction option turned off, the gas would reach the walls of the container within five cycles of a K3 run, or within .04 microseconds of problem time. The CP time for a K3 run to this point was approximately three seconds which greatly expedited the turn-around time for a job. Results were deemed satisfactory when the following was observed:

- o Total momentum of the system to the time of boundary contact was zero;
- o Velocities, temperatures, pressures, etc., in cells of symmetrically opposite positions were of the same absolute value and with the correct sign;
- o Mass was conserved, i.e., mass did not leak through the reflecting walls of the container;
- o Total energy of the system was conserved to a few percentage points error;

- o Values for cell parameters in the K = 4 plane agreed with a CSQ benchmark run throughout the history of a run.

Variations on this configuration were run to test the reflective-transmittive boundary options, i.e., some walls were reflective while others were transmittive, allowing mass to flow out of the problem. Comparisons were made with CSQ benchmark runs and with previous K3 runs to determine that when opposite walls were transmittive or reflective, symmetry was preserved and that results were independent of which opposite boundarys were transmittive.

Another variation of this configuration was formulated to test out the elastic-plastic package of routines. In this configuration, the gas was replaced with a solid block of aluminum and given an initial velocity in first the minus-X direction, then, in another run, in the plus-Y direction, etc., and results of the impact with the walls of the problem examined. Again, results were satisfactory when symmetry was preserved and when they agreed with CSQ benchmark runs.

2. Aluminum Block - Steel Ball Impact Problem

This problem was an attempt to duplicate a previous CSQ calculation where CSQ was run to simulate an experiment conducted at Arnold Engineering Development Lab, Tulahoma, Tennessee. Since the CSQ run gave excellent results, in complete agreement with empirical data, it was expected that K3 should give comparable results before it was certified operational. The following paragraphs present the history of the K3 run and comparisons with the original CSQ run.

The problem as initially configured is shown in Figure A-2a for CSQ and Figure A-2b for K3 (neither figure is to scale). Units are in centimeters. CSQ was run using the cylindrical geometry option, therefore the aluminum block (and steel backing) as well as the steel ball were taken as figures of revolution about the Y-axis with radii of 15.24 and .9166 centimeters, respectively. K3 was run using the only available option, Cartesian geometry, with reflective boundarys on the X = 0 and Z = 0

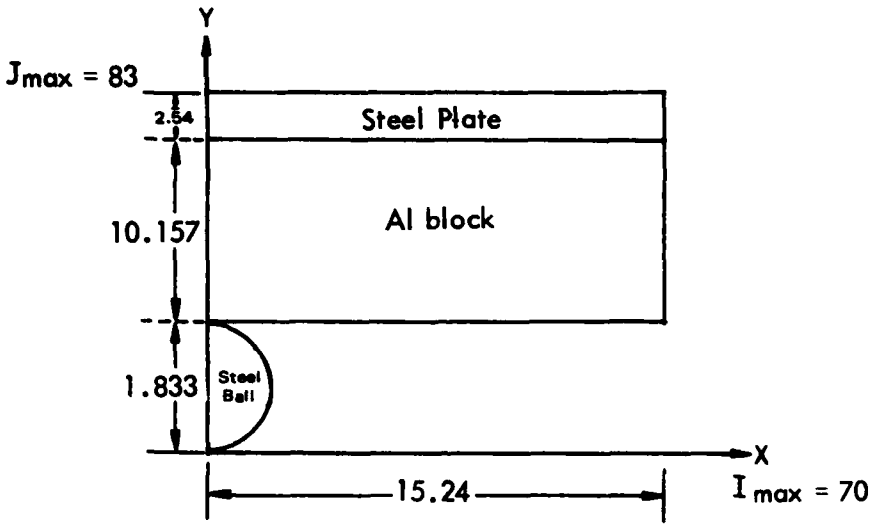


FIGURE A-2a

CSQ AL BLOCK/STEEL BALL PROBLEM

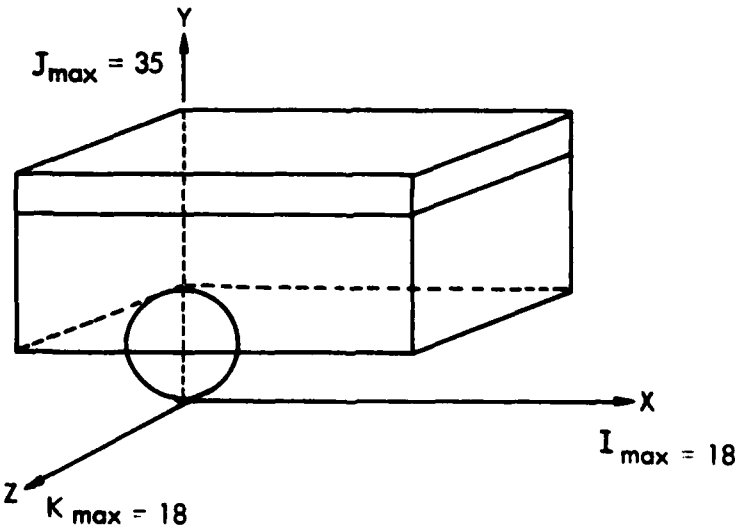


FIGURE A-2b

K3 AL BLOCK/STEEL BALL 3-D PROBLEM

planes (Y - Z plane and X - Y plane). This essentially reduced the problem configuration to one-fourth of the physical geometry, i.e., only that part of the block and sphere which is in the positive-X, positive-Z quadrant is simulated. The dimensions for the K3 configuration were identical to those for CSQ.

For the CSQ run, there were NVAR = 16 variables stored for each cell in the problem*, or a total of I_{max}*J_{max}*NVAR = 92960 words. K3 was zoned with I_{max} = 18, J_{max} = 35, and K_{max} = 18, and with NVAR = 17, used a total of 192,780 words of storage for cell variables. This particular zoning kept the required size of cell storage below the size which, if exceeded, would force some storage onto disk and increase the run time. Though the zoning was more coarse for the K3 problem, previous studies using CSQ with fine and coarse grids showed the size of the zones had little effect on the results for problems of this type, as long as the spacing was judiciously chosen.

The K3GEN inputs for this problem are shown in Figure A-3a. Note the velocity of the ball is 4.995×10^5 cm/sec in the +Y direction. The K3 inputs are shown in Figure A-3b. K3 was set to run 200 cycles, which translated to approximately 16 μs (computer time required was slightly over one-half hour of CP time). The restart tape produced by K3 was then input to K3PLT and selected dumps plotted. Figures A-4, A-5 and A-6 show the title, mesh and dot scale frames produced (by user options) by K3PLT. As the mesh frame indicates, the reflective option in K3PLT was chosen, and the plot scale chosen so $-8.0 \leq x \leq 8.0$ i.e., only a portion of the aluminum block/steel backing is shown, effectively enlarging the area of interest. Figure A-7 shows the configuration of the K3 problem at time zero, K = 1 plane only.

---

* Three materials were defined, since the steel backing and steel ball were different alloys. In K3, in order to reduce NVAR, the steels were assumed to be alike.

```
 STEEL BALL/AL PLATE  3-D TEST
    2              -1   -2
 -1        STEEL 1020                                          -1.        -1.
1.         4.        7.8335                        -4.5475 E5 2.04
2.0285               6.0733 E10 .1464

26.  1.
 -2        AL 1100                                             -1.        -1.
1.         4.        2.71                          -5.339  E5 2.13
1.35                 2.07   E11 .06899

13.  1.
                                        21   15   23    1
1.0        2.0       1.0

1.   1.   1.              1.
   41   18 .2        16.
   40
   51   15 .2        3.0
   51   20 .2        12.
   50
   61   18 .2        16.0
   60
   73    5           1     STEEL BALL
   79     0.         .9166                 .9166     .9166     .9166
   93                4.995   E5
   90
   71    5           2     AL PLATE
   79                1.833                 15.24     11.99     15.24
   90
   71    5           1     STEEL BACKING
   79                11.99                 15.24     14.53     15.24
   90
   70
```

FIGURE A-3a. K3GEN INPUTS

```
        STEEL BALL/AL PLATE  3-D TEST
                    200   -1    -1        200                    2
              1.0        2.0              1.0   60.0              .5  1.05
                 0         50
                 0        200
              -5.175+09 -8.970+08                      1.0
                 1    2  -1.000+9
               3.312+09              .26
               3.450+08              .30
```

FIGURE A-3b. K3 INPUTS

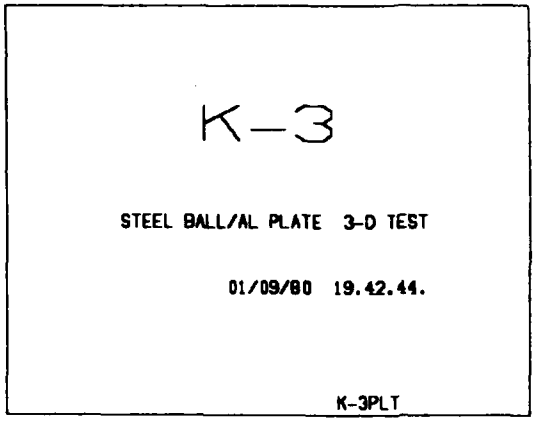


Figure A-4
K3PLT Title Frame

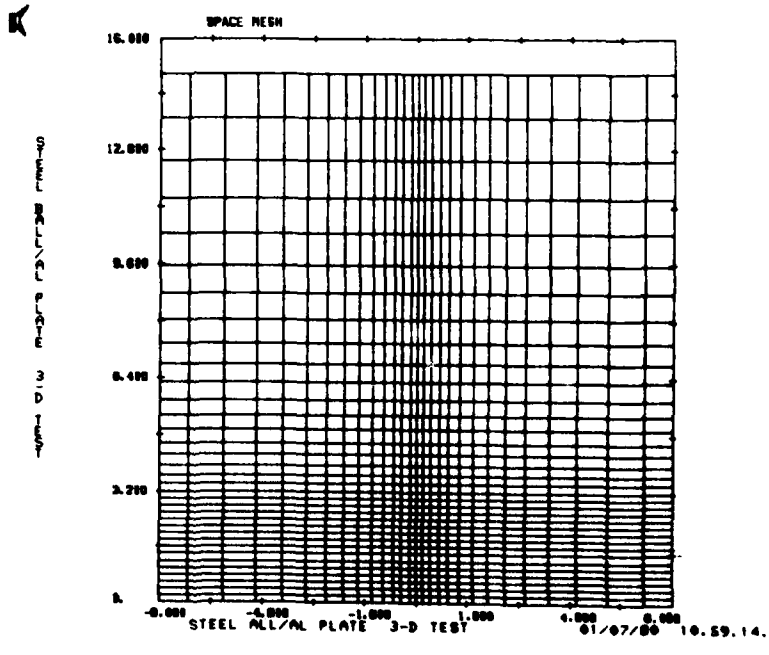


Figure A-5
K3PLT Mesh Frame

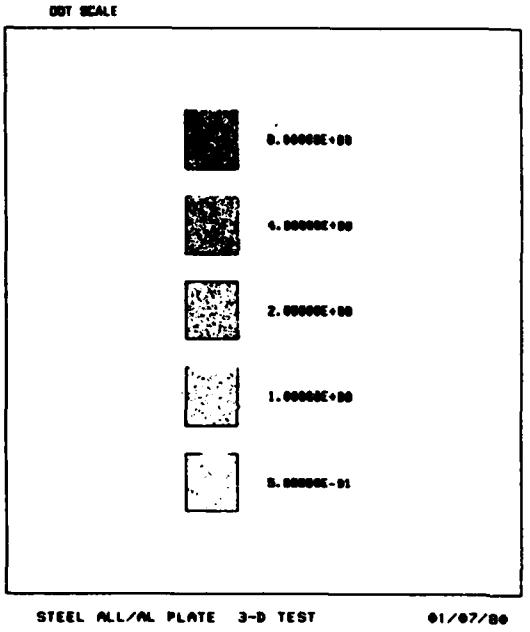


Figure A-6
K3PLT Dot Scale Frame

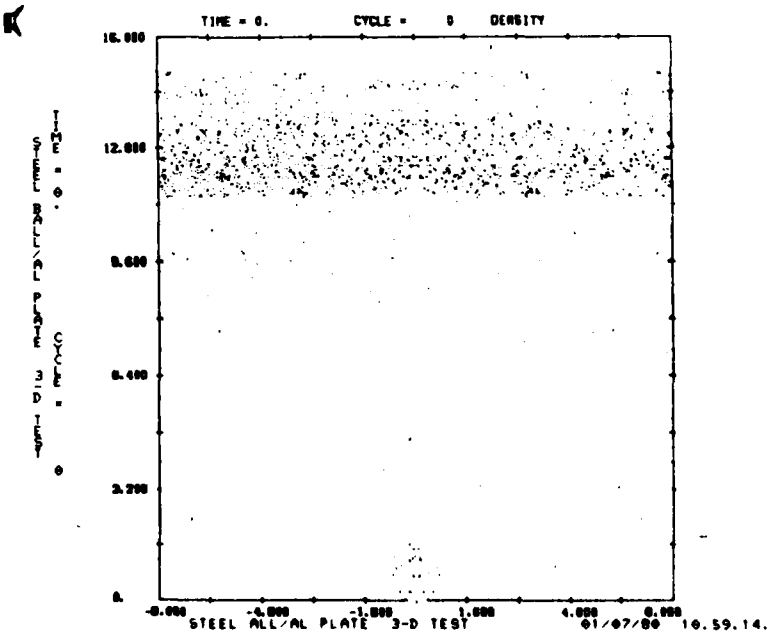


Figure A-7
Material Density Plot
at Time = 0.0
K = 1 Plane Only

Figure A-8 shows the K = 1 plane at problem time 4.5 μs, and Figure A-9 shows the K = 1 through 5 planes at the same time (the K-planes overlay, or are superimposed upon, previously plotted K-planes, hence the darker the plots, showing increased density). Material density for cycle 136, problem time 7.5 μs, is shown in Figures A-10 through A-12. Figure A-10 shows the K = 1 plane, Figure A-11 K-planes 1 through 8, and Figure A-12 K-planes one through 15. Figures A-13 and A-14 show the material density for the K = 1 plane and K = 1 through 8 planes, respectively, near the end of the problem. Figures A-15 and A-16 show a different view of K3 results for this problem time. Here, only the right-half of the configuration is shown (positive X, Z quadrant) rotated -30 degrees about the X-axis and +45 degrees about the Y-axis. Both show an increasing number of K-planes. Figure A-17 gives a schematic representation of these views for better interpretation. Note the area of impact is on the back-left corner of the material block.

The size of the cavity predicted by CSQ and K3 at approximately 10 μs is shown in Figure A-18. Considering there is a difference in time of 1.14 μs between the CSQ plot and the K3 plot, and there is still appreciable movement in the mass, the shapes of the cavities are in good agreement.* The lip formed on the cavity boundary, however, is somewhat smaller in K3 than it is in CSQ. An examination of the total output from K3, i.e., an examination of K-planes away from the K = 1 plane revealed that the lip is larger as one progresses away from the reflective boundary, and is in agreement with CSQ results. This result may be due to conditions imposed by the boundaries and the problem configuration (size of zones), but further explanation must await a detailed study. The mass in the extremes of the lip is very small though, representing fractured or vaporized material no longer connected to the bulk of the aluminum block, and therefore has little if any effect on this particular problem.

---

* The plotted points are shown with error tolerances which indicate the width of a cell at the point and the uncertainty of locating the exact mass boundary. Note the K3 cell widths are much greater than the CSQ cell widths due to the coarseness of the K3 grid.

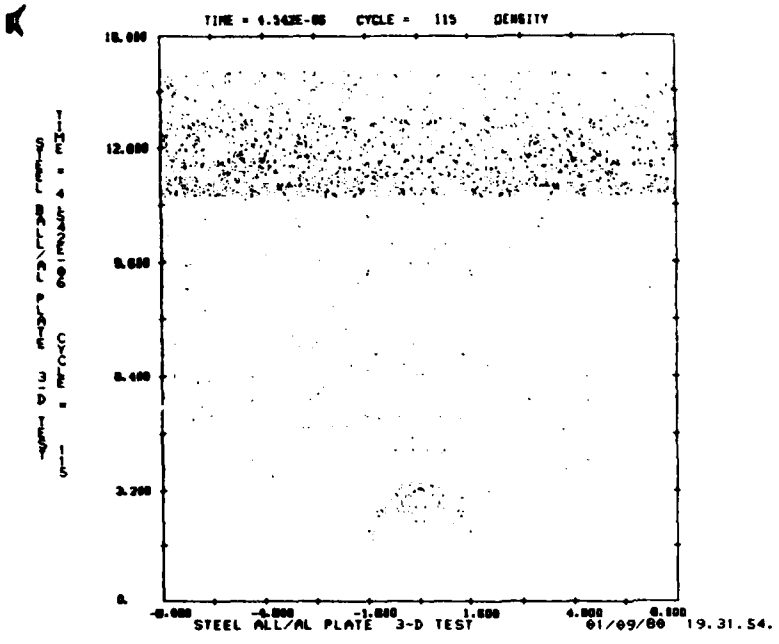


Figure A-8
Material Density Plot
at Time = 4.5 μs
K = 1 Plane Only

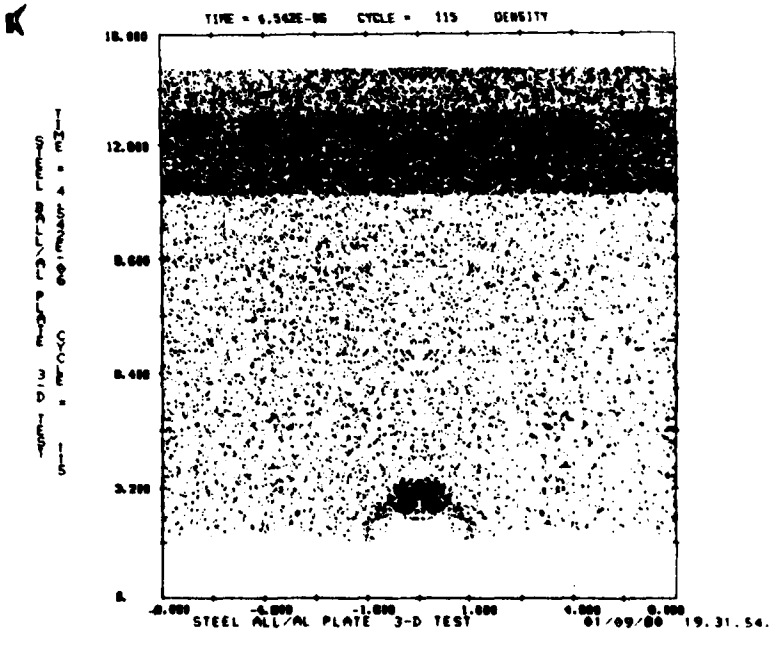


Figure A-9
Material Density Plot
at Time 4.5 μs
K = 1 through 5 Planes

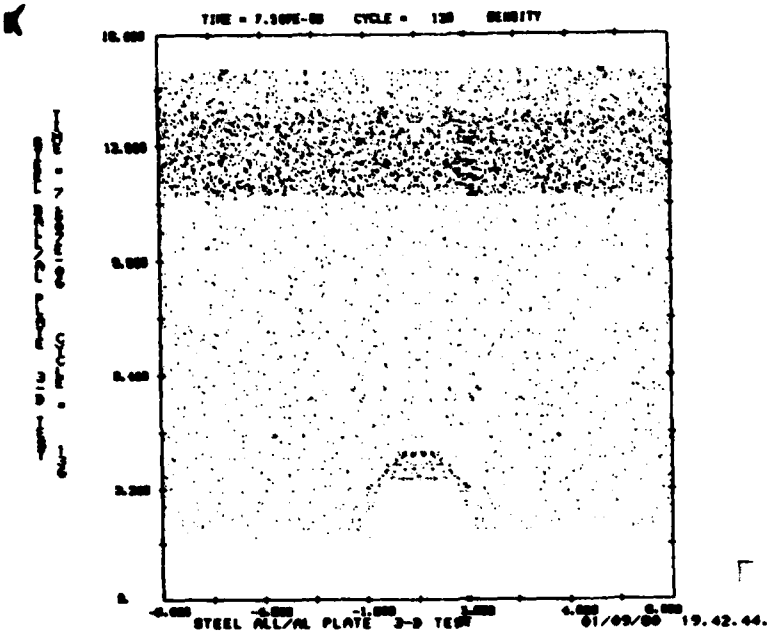


Figure A-10
Material Density Plot
at Time = 7.5 μs
K = 1 Plane Only

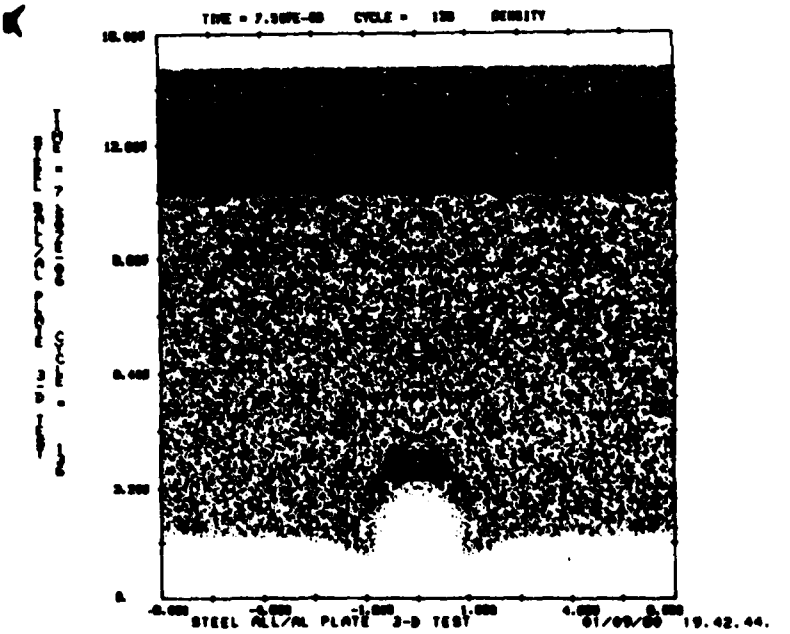


Figure A-11
Material Density Plot
at Time = 7.5 μs
K = 1 through 8 Planes

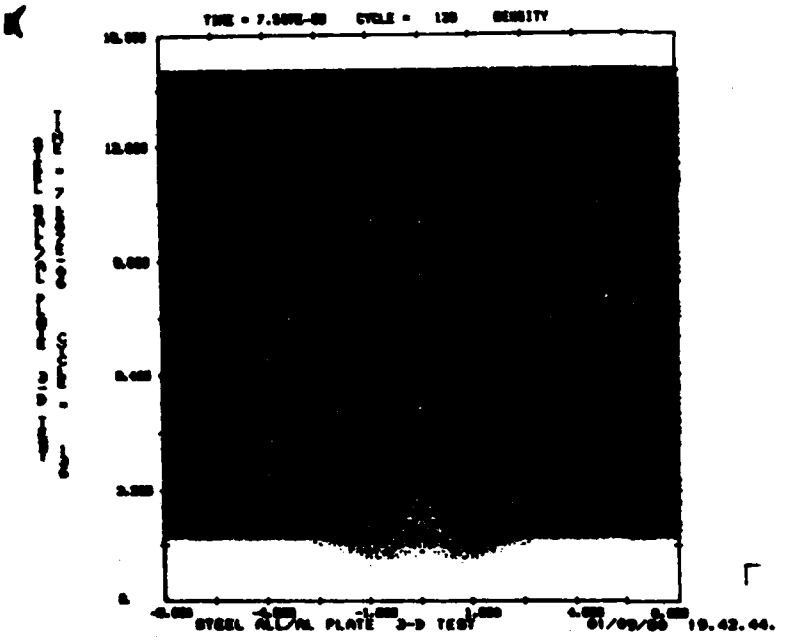


Figure A-12
Material Density Plot
at Time = 7.5 μs
K = 1 through 15 Planes

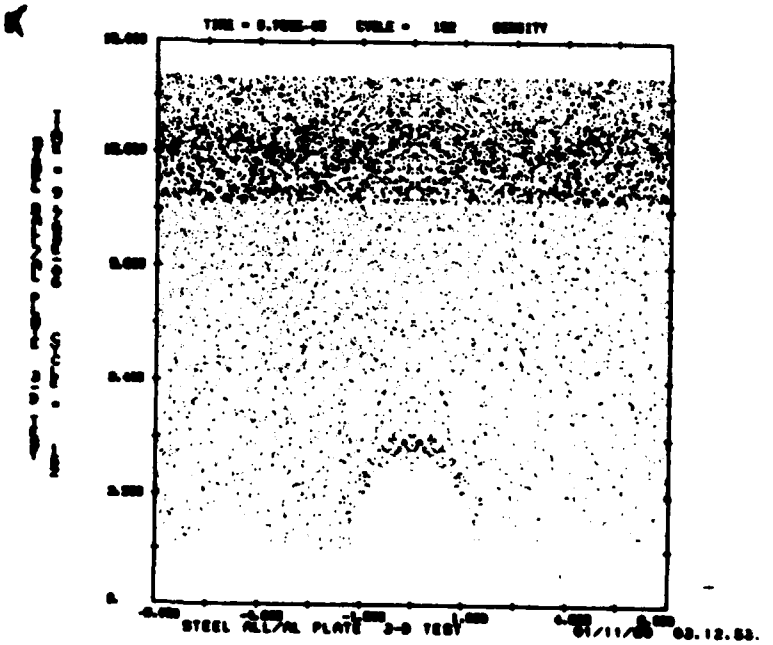


Figure A-13
Material Density Plot
at Time = 9.8 μs
K = 1 Plane Only

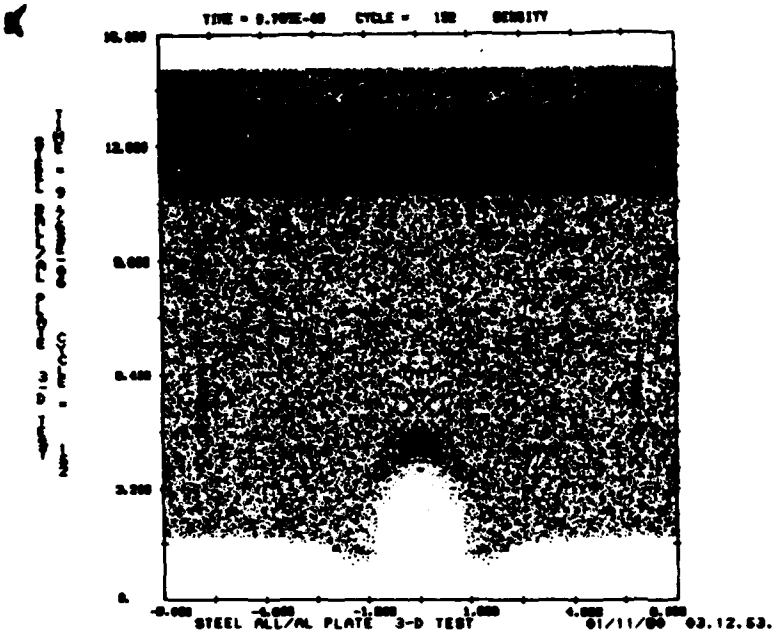


Figure A-14
Material Density Plot
at Time = 9.8 μs
K = 1 through 8 Planes

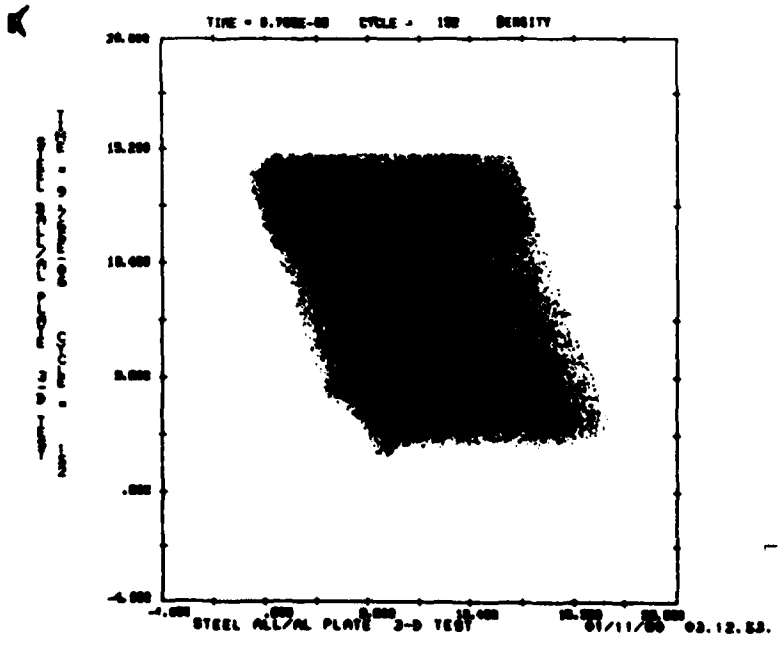


Figure A-15
Material Density Plot
at Time = 9.8 μs
Rotated About X, Y Axis

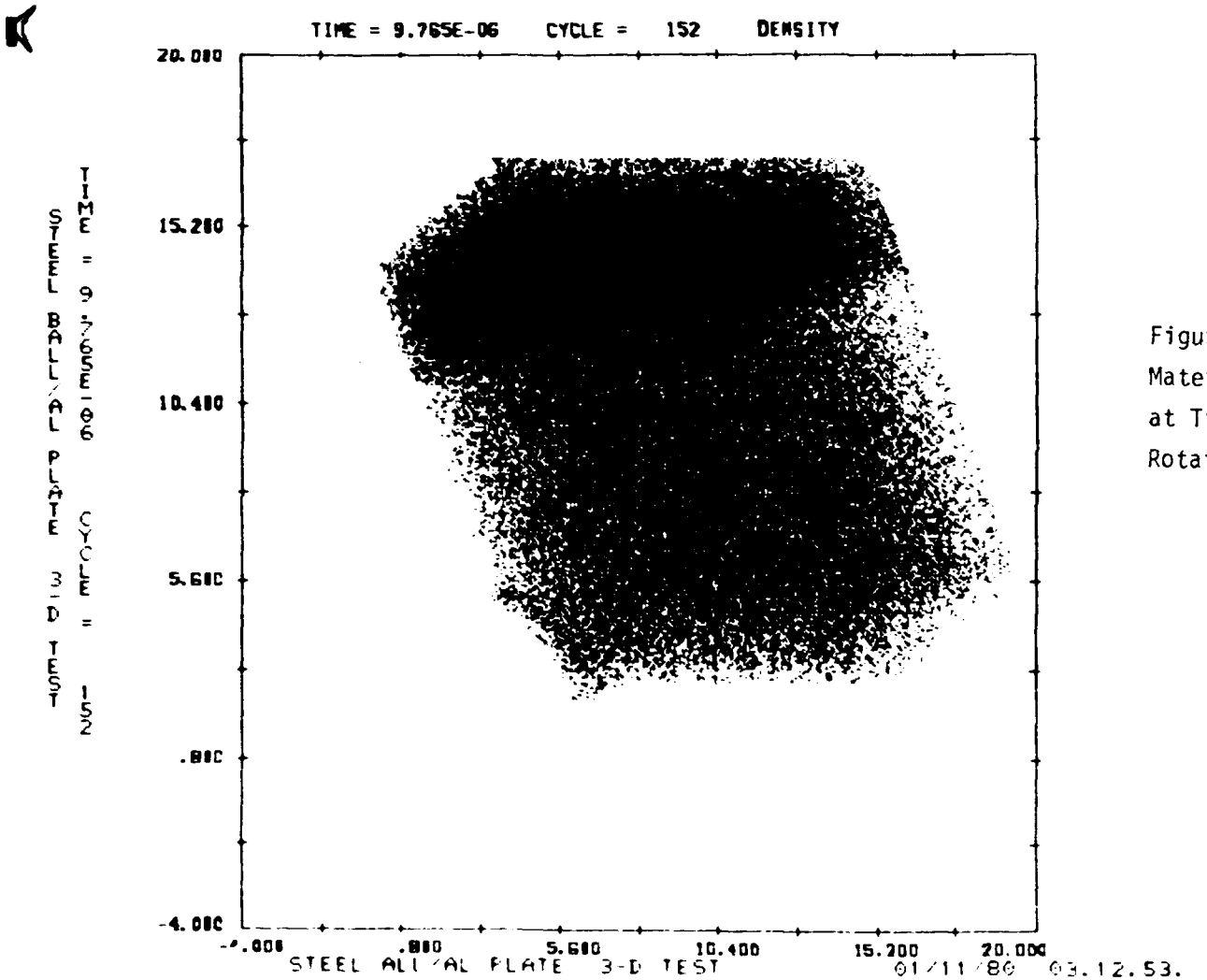


Figure A-16
Material Density Plot
at Time = 9.8 μs
Rotated about X,Y Axes

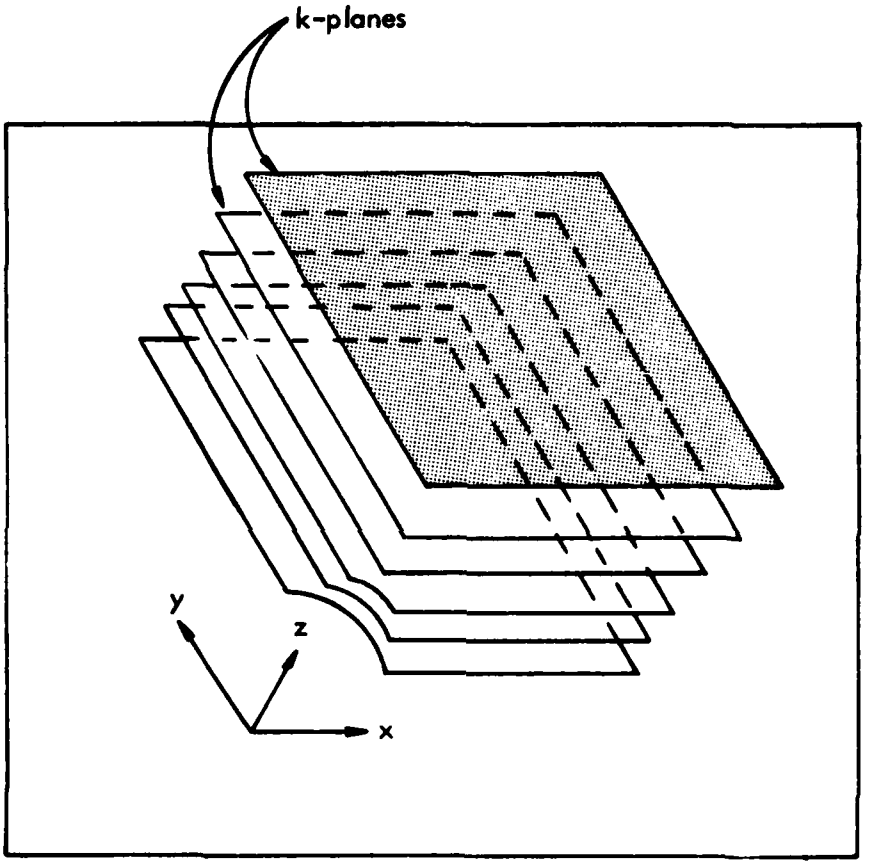


FIGURE A-17

SCHEMATIC REPRESENTATION OF FIGURES A-15 AND A-16

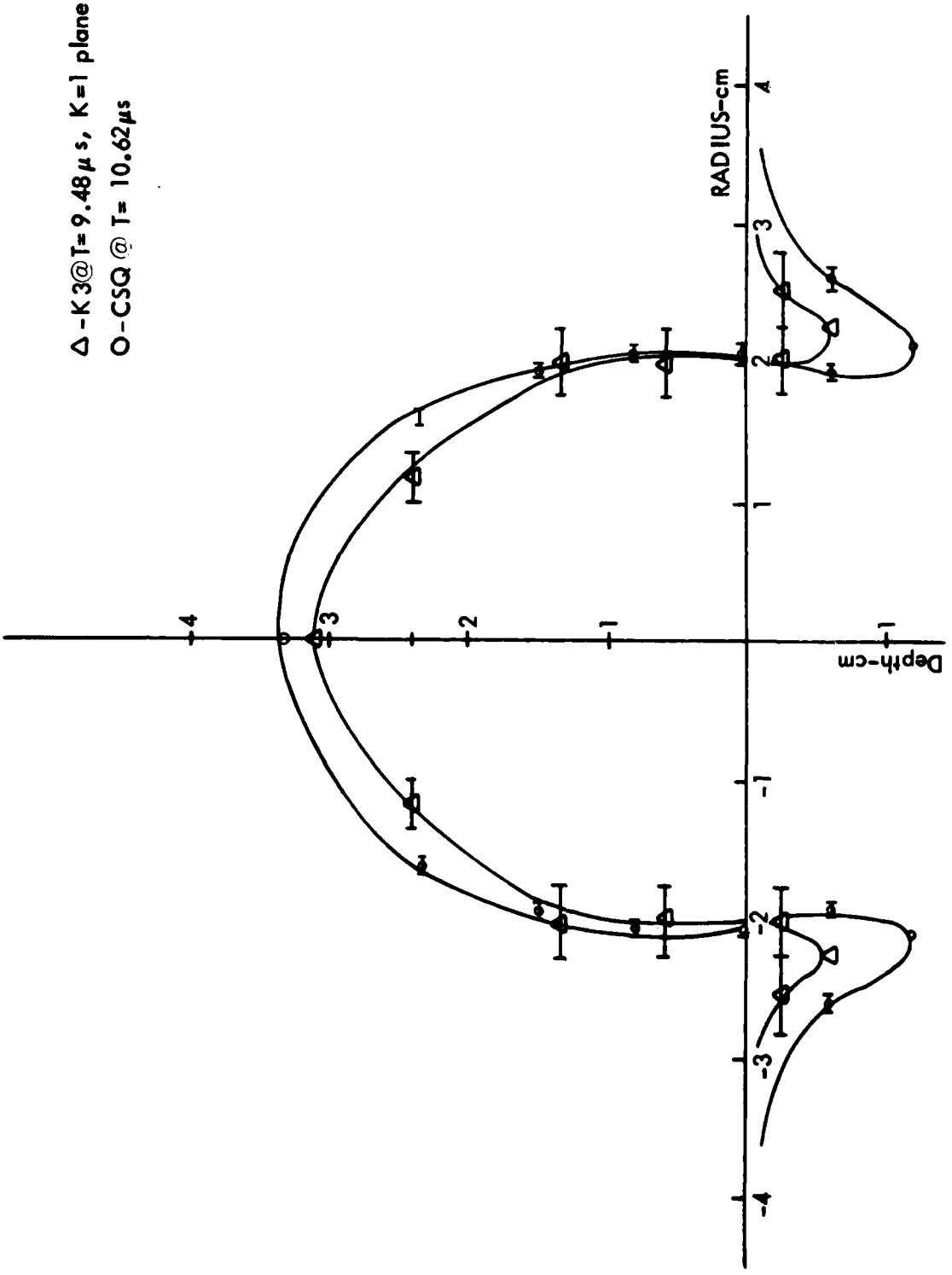


FIGURE A-18

CAVITY SHAPES FROM CSQ AND K3 CODE

Figure A-19 shows the comparative cavity sizes at or near 16 μs problem time. With a close match in problem times between K3 and CSQ, the cavity sizes are also in close agreement. Though the cavity lips are more closely matched than in Figure A-18, there is a different shape. Again, this may be due to the coarseness of the grid.

While the CSQ code was run out to almost 100 μs, K3 was terminated at this point since little information could be gained by running it further with this particular zoning. Future work on the code will be directed at incorporating the rezoning feature now in CSQ into K3, thereby allowing problems of this type to be run further with a reduced execution time.

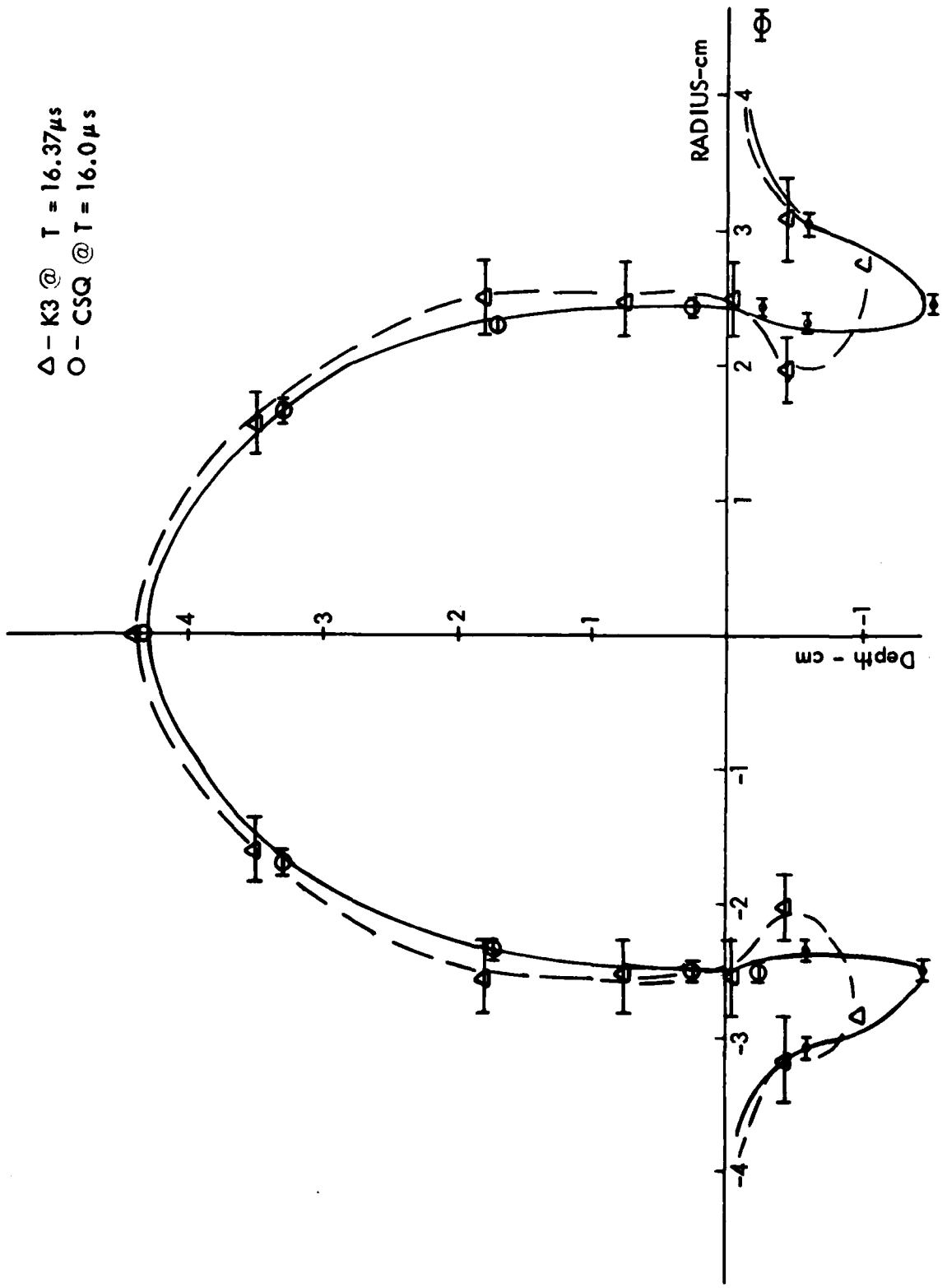


FIGURE A-19

CAVITY SHAPES FROM CSQ AND K3 CODE

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